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Description of the Strategic High-Altitude Atmospheric Radiation Code (SHARC)

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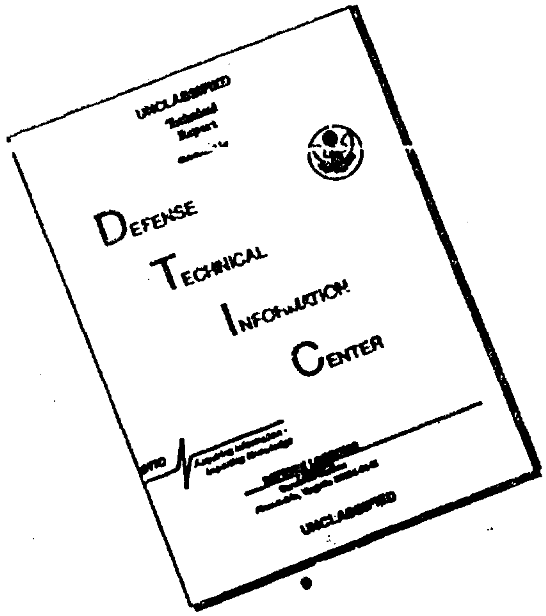

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This report describes an upgraded version of the Strategic High-Altitude Radiance Code, SHARC-2. SHARC calculates atmospheric radiance and transmittance over the 2-40 µm spectral region for arbitrary paths within 50 and 300 km altitude, including space viewing. It models radiation due to NLTE (Non-Local Thermodynamic Equilibrium) molecular emissions which are the dominant sources at these altitudes. This new version, which is now ready for distribution, has been upgraded to include a fully integrated auroral model with time-dependent chemistry, extention down to 50 km altitude, and radiation from the minor isotopes of CO_2. In addition, there have been numerous internal upgrades to the various modules. These include a Voigt lineshape for the radiative excitation module; embedding of the auroral region into a quiescent atmosphere; and improvements in the radiation transport algorithms.

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1. INTRODUCTION

This user's manual is for the second release of the Strategic High-altitude Atmospheric Radiation Code (SHARC-2). This manual will emphasize the use of SHARC-2, giving the user detailed code implementation instructions and sample interactive sessions. Just like the first release of SHARC,[1] henceforth called SHARC-1, SHARC-2 predicts infrared (IR) atmospheric radiation and transmittance in the 2-40 μm spectral region and includes important bands from the major isotopes of NO, CO, H_2O, O_3 and CO_2. There are however several upgrades which have been incorporated in SHARC-2. They include:

- the atmosphere can now be partitioned into one or two distinct regions, called extended and local regions,
- the model now includes time dependent auroral chemical kinetics and spectroscopy for CO_2, NO and NO+,
- the minor isotopes of CO_2 are now included in the species which SHARC currently supports, and
- the lower altitude has been moved from 60 to 50 km.

These upgrades allow SHARC-2 to simulate time dependent auroral phenomena by placing the simulated aurora in a local region and surrounding the local region with an ambient atmosphere. The geometry module has been upgraded to inform the user if the selected line-of-sight (LOS) intersects a local region. This information aids the user in selecting a LOS which samples the aurora, if such a LOS is desired. This manual discusses the new features found in SHARC-2 and reviews some features which SHARC-2 and SHARC-1 have in common.

Generally above an altitude of 60 km collisional excitation and de-excitation processes between molecules occur on a time scale comparable

to radiative decay. This leads to a condition of Non-Local Thermodynamic Equilibrium (NLTE) where the various degrees of vibrational, rotational, and translational freedom cannot be characterized by a single temperature. In this regime the concept of temperature, which implies a Boltzman distribution of excited-state populations, is invalid, and the explicit molecular excited-state populations need to be determined. In order to compute these populations, a comprehensive model is required which incorporates all the important physical processes which for this problem include: (1) collisional excitation, de-excitation, and energy transfer; (2) chemical production of excited-state molecules; (3) radiative decay; (4) external source excitation due to solar and earthshine pumping; (5) internal radiative excitation due to emission and absorption by molecules within the atmosphere; and (6) molecular excitation resulting from time-dependent chemistry due to high energy electrons found in auroras. All these effects are incorporated in SHARC-2.

SHARC-2 was developed as a modular code so that models and model parameters can be easily modified or upgraded as additional data and/or better models become available. The present modules include input, ambient chemistry, time dependent auroral chemistry, radiative transport, geometry, and output. The input module is interactive, menu-driven and checks all input parameters for validity before continuing with the calculation. It is through the input module that a user sets up the simulation.

A typical simulation could be the radiance calculation for a LOS which passes through a class III auroral region nested in an quiescent atmosphere. The input module prepares the inputs which are required by the rest of the code. The next step is calculation of the excited-state populations. This is accomplished in the chemistry modules: ambient and auroral. The ambient population module iterates between a generalized chemical kinetics module that calculates excited-state populations due to solar and earthshine excitation and a Monte-Carlo based radiative transfer model that calculates radiative excitation and energy transfer between

atmospheric layers. The auroral module is based on the AFGL AARC code[2] and solves the time/energy dependent rate equations to calculate the secondary electron distributions and reactive/energy transfer processes, and the subsequent enhancement to various CO_2, NO and NO+ vibrational states. The auroral module requires a set of ambient populations to start the calculation, which couples the ambient and auroral regions. The geometry module determines the species column densities for each layer traversed by the user's requested path. The radiative transport module then calculates the radiance along the path for each molecular excited state. The calculation is done on a line-by-line basis in that the total radiation from each line is calculated using a single-line equivalent-width formulation that incorporates a Doppler-Lorentz (Voigt) lineshape. Finally the results are passed to a separate plotting package which prepares a spectral plot of the calculated radiance.

2. PROGRAM OVERVIEW

There are three major components of the overall SHARC software package, and these are indicated in Figure 1. The INTERPRETER, which is a modified version of that furnished with the Sandia CHEMKIN code,[3] prepares the differential equations for the chemical/kinetic reaction scheme. This module is run only when changes are made to the reaction scheme or its associated rate constants. The SHARC chemistry modules are composed of many sub-modules, each of which models a specific physical process. These modules, ambient and auroral, utilize the differential equations set up by the INTERPRETER and associated atmospheric and spectroscopic data to determine spectral radiances for arbitrary spectral

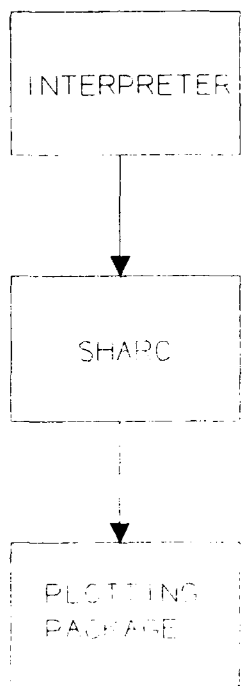


Figure 1. Major Components of SHARC.

regions, molecular emitters, and viewing geometries. Finally, a PLOTTING package is provided which allows the user considerable flexibility to vary the display format of the spectral radiance plots. The functions of each of these modules are described in the following sections.

2.1 The INTERPRETER Program

The SHARC CHEMKIN module computes the steady-state and time-dependent number densities of vibrationally excited atmospheric species from a set of chemical kinetics/reaction mechanisms. The chemical kinetics mechanism describes molecular formation, all forms of vibrational energy transfer, and the absorption of solar and/or earthshine radiation. SHARC's access to the chemical kinetics mechanism and associated input (i.e., energy transfer or reaction rate constants) is provided by a program called the INTERPRETER. The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism (written in a manner just as a chemical kineticist would write it), and creates a binary "linking" file which contains all of the kinetics information. The SHARC INTERPRETER is based entirely on and includes subroutines directly from the Sandia Livermore INTERPRETER code which is provided with the CHEMKIN code.[3] The Sandia CHEMKIN package is described as "a general-purpose, problem-independent, transportable, FORTRAN chemical kinetics code."[3] The SHARC INTERPRETER is a modified Sandia interpreter from which information on elements in the periodic table and the thermodynamic data base (useful for combustion reactions), extraneous for our application, has been removed.

Once the chemical kinetics mechanism has been formulated, the INTERPRETER provides the vehicle by which the information is transferred to the CHEMKIN module in SHARC. The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism in a manner that is just as would be written by a chemical kineticist; it then translates this information into the appropriate differential rate equations. To be more

specific, consider I irreversible kinetic (energy transfer or reactive) processes, each given in the general form

$$\sum_{k=1}^{K} \nu_{ki} C_k \xrightarrow{k_i} \sum_{k=1}^{K} \nu'_{ki} C_k \quad , \tag{1}$$

where the stoichiometric coefficients ν_{ki} are integers; the C_k is the chemical symbol for the k^{th} species; and k_i is the rate constant for the ith process. The INTERPRETER reads this symbolic description of an arbitrary chemical kinetics mechanism and provides the data necessary to translate the mechanism into the appropriate differential equations

$$\frac{dw}{dt} = \sum_{i=1}^{I} (\nu'_{ki} - \nu_{ki}) k_i \prod_{k=1}^{K} [C_k]^{\nu_{ki}} \quad . \tag{2}$$

All the variables defined in Equations (1) and (2) are written into a binary "linking" file. Although this example is shown for irreversible processes, it should be noted that SHARC-2 allows the use of reversible vibrational to translational processes. However, reversible vibrational to vibrational energy exchange processes must still be explicitly entered as irreversible reactions in the forward and reverse directions. The INTERPRETER only has to be run once for a given kinetics mechanism and data base. The "linking" file is then saved and used by SHARC for all subsequent calculations. Of course, if the kinetics mechanism or data base is changed, the INTERPRETER has to be rerun.

2.2 SHARC

The schematic shown in Figure 2 illustrates the calculational sequence for SHARC. Except for the PLOTTING and the INTERPRETER modules, which are run separately, all the modules are called by the MAIN program.

The interactive input module queries the user for the parameters needed by the rest of the code.

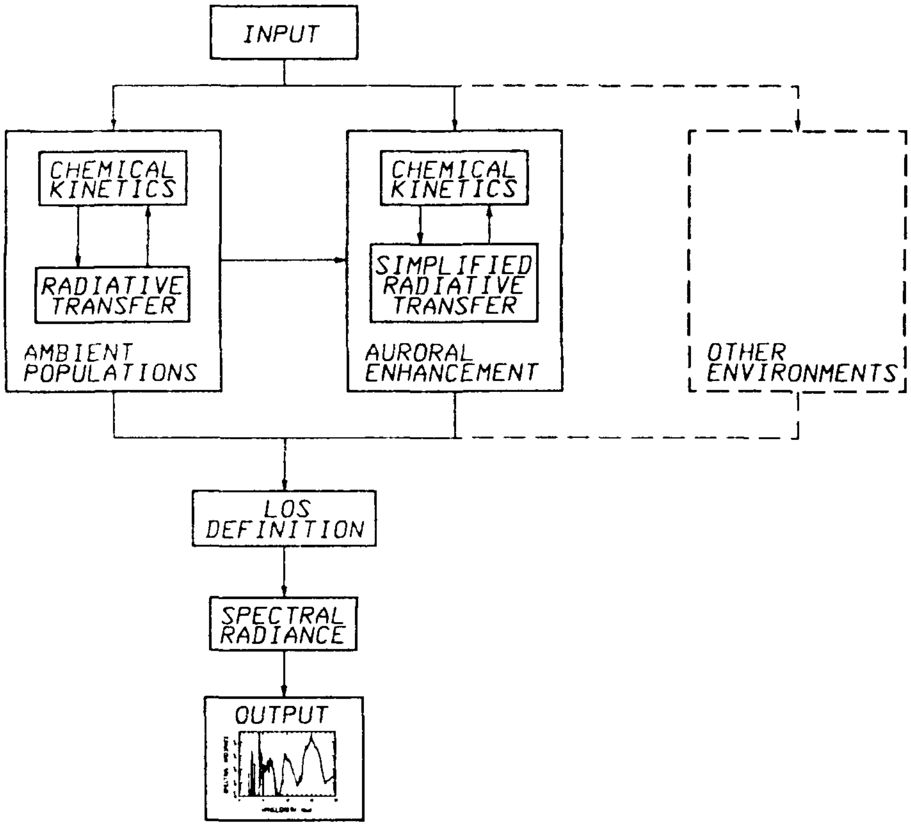


Figure 2. Calculational Sequence for SHARC.

The ambient atmospheric chemistry module includes two components, a chemical kinetics module (CHEMKIN) and a radiative transfer model (NEMESIS). They calculate the NLTE populations for the various molecular excited and ground states. CHEMKIN calculates excitation due to chemical reactions and energy transfer processes plus solar and earthshine pumping. NEMESIS then calculates changes in the excited-state populations due to radiative transfer between molecules within the atmosphere. The auroral chemistry module calculates the auroral enhancement of the ambient

populations. This module uses a time-dependent chemical kinetics module (CHEMKIN) and a simplified radiative transfer model based on Kummer's Q_W approximation[4] to calculate the radiative transfer between molecules within the aurora.

The GEOMETRY module determines the line-of-sight (LOS) trajectory parameters for the viewing geometry requested by the user. It uses the density profiles calculated by population modules to determine the LOS column densities for each excited state. Arbitrary paths between 50 and 300 km are allowed, including limb viewing from space, vertical and horizontal paths, and slant paths of arbitrary length and direction. This module also alerts the user if the LOS "misses" the localized region, such as an aurora.

The SPCRAD module utilizes the geometry information provided by GEOMETRY and the state populations along with a molecular spectroscopic data base to determine the LOS spectral radiance.

2.2.1 The INPUT Module

The INPUT module is used to interactively change input parameters required for a SHARC calculation. The module is used to modify and enter input parameters in an interactive query-menu mode. When SHARC is used in the batch or background mode, a previously created input file must be used. In the interactive execution mode, SHARC will look for the input file called "SHARC.INP". This file contains the user-supplied input parameters for SHARC (several of these files are supplied on the SHARC computer tape and discussed in the test case section of this manual). If "SHARC.INP" is not found, the input module will use a set of default values for all input parameters. Once SHARC has a set of input parameters, the input module displays the top-level input menu. The query-style menus used in the input module were modeled after the input menus used in the AFGL Auroral Atmospheric Radiance Code (AARC).[2] The top-level menu looks like this:

```
STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

REVIEW OR MODIFY INPUT PARAMETERS

1) TITLE FOR CALCULATION
2) REGION DEFINITION
3) LOS GEOMETRY
4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
5) SOLAR ZENITH ANGLE
6) OUTPUT DATA
7) STANDARD SET-UP FOR FILE NAMES

8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
9) EXIT WITH NO UPDATE OF DEFAULT FILE

 ENTER OF ITEM TO BE CHANGED OR
 0 TO CONTINUE
```

The user can enter a number from 1 to 7 to enter a submenu on topics 1 through 7. The submenu will start by reviewing the current parameter values found in SHARC.INP, and the user can then select a parameter to be changed. The value is then changed simply by typing in the new value and then entering a 0 will return the user to the submenu level. Entering another 0 will return the user to the main menu. At this stage the user can enter another submenu by inputing a value from 1 to 7 or, by entering a value of 8, the user can exit the input menu and update the "SHARC.INP" file for a batch calculation. Entering an 9 will exit the SHARC calculation without changing the "SHARC.INP" file (used to quit SHARC when many input parameters have been incorrectly entered), and entering a 0 will allow SHARC to continue interactive execution. A more complete example of an interactive input session is described in Section 4.2.

Changes made to input parameters will be saved in the "SHARC.INP" file. The first parameter in "SHARC.INP" determines whether SHARC is to be run in an interactive or batch/background mode. When this parameter is a

1, SHARC will run interactively and enter into the input module. When this parameter is 0, SHARC will execute in a batch or background mode and skip the input module. This parameter is set to a value 1 after complete execution of SHARC so that the default mode for SHARC is the interactive mode. If a batch run is desired, this parameter can be changed by editing the "SHARC.INP" file, or one can exit SHARC with option 10 which prepares "SHARC.INP" for batch execution, i.e., the mode parameter is set to 0.

2.2.2 The Ambient Population Module

The first component of this module is CHEMKIN. It computes the steady-state number densities of vibrationally excited atmospheric species from a set of chemical kinetics/reaction mechanisms for each atmospheric layer. Again the subroutines comprising the CHEMKIN module are based on those included in the Sandia Livermore CHEMKIN package.[3]

The CHEMKIN module uses the input read from the "linking" file (species identification, stoichiometric coefficients, and rate constant parameters) to construct the steady state equations for the vibrationally excited states

$$\sum_{i=1}^{I}(\nu'_{ki}-\nu_{ki})k_i\prod_{k=1}^{K}[C_k]^{\nu_{ki}} = 0 \quad . \tag{3}$$

The variable definitions are identical to those defined in Equation (2). In general, solving Equation (3) for the vibrationally excited-state densities requires a nonlinear equation algorithm. However, using the assumption that the ν_{ki} of the vibrationally excited species (i.e., the unknowns in the problem) are unity, Equation (3) simply reduces to a set of linearly independent algebraic equations for the N unknown excited-state number densities. This assumption is not overly restrictive and has been used previously in atmospheric radiation models.[2,4] The information necessary to solve Equation (3) is simply the atmospheric species number

densities and the kinetic temperature from which the rate constants are computed. SHARC then uses a lower/upper (LU) decomposition algorithm to solve Equation (3) for the number densities.

The second component in the ambient population module is NEMESIS (Non-Equilibrium Molecular Emission and Scattering Intensity Subroutine) which computes the enhancement of the atmospheric excited-state layer populations due to layer radiative self-trapping and layer-layer radiative pumping. Some molecular bands, in particular the 4.3μm CO_2 band, are optically opaque to emitted radiation. Photons emitted in these bands may be absorbed and emitted many times before either escaping the atmosphere or becoming collisionally quenched.

The overall approach for determining the enhanced excited-state level populations involves:

- determination of the steady-state layer source populations which includes excitation by external light sources, sun and earthshine, and molecular collisions, and de-excitation by radiative decay and collisional quenching;
- determination of the first-order population enhancement using a Monte Carlo simulation of the initial source photon emissions and their subsequent absorption or escape; and
- determination of the total enhanced populations using a recursive orders-of-enhancement approximation which is initialized by the Monte Carlo first-order results.

The source populations include all sources of excitation exclusive of the internal atmospheric radiative effects of layer self-trapping and layer-layer pumping. CHEMKIN is used to generate the source populations that are then input into NEMESIS. The key results from the Monte Carlo simulation are the first-order enhancements and the probabilities that a photon emitted from a layer "i" will create a new excited-state in a layer "j". This simulation involves sampling over the initial emission position, emission direction, emission frequency, emission line strength, and length

of travel. The contribution of each succeeding order-of-enhancement is determined recursively by

$$(P_k) = (P_{k-1})(W) \quad , \tag{4}$$

where (P_k) is the kth-order layer population enhancement matrix, and (W) is the layer-layer absorption probability matrix. Both (P_1) and (W) are determined by the first-order Monte Carlo calculation.

The end result of each NEMESIS calculation is the total excited-state population distribution for a pair of vibrational levels, where the lower level of each pair may itself be an excited level. A cycling procedure between CHEMKIN and NEMESIS is used to step up the vibrational energy ladder until the top of the ladder is reached. Finally, the ambient populations are passed to the SPCRAD module for line-of-sight spectral radiance computation.

2.2.3 The Auroral Population Module

The primary function of the AURORA module is to perform a time dependent calculation to determine auroral species number densities as a function of altitude. The Gear method for stiff differential equations is used to numerically integrate the chemical kinetic rate equations describing auroral chemical and energy transfer processes. This integration package is supplied as part of the Sandia CHEMKIN code[3] and thus has been extensively applied to many different types of scientific problems.

In addition to the normal SHARC inputs, the following inputs are required to execute the AURORA module:

- definition of the strength and duration of the aurora,
- specification of the chemical kinetics mechanism for the selected emitter, including primary and secondary electron processes.

The primary electron deposition model used in SHARC is based upon the work of Grun, Rees, and Strickland and has been discussed in some detail in the AARC manual.[2] Routines describing the energy deposition are based upon those used in AARC. The ion pair production rate is then obtained from the energy deposition rate by assuming that 35 eV are required to produce an ion pair. Default parameters for selecting several different strength auroras are contained in SHARC, although the user can easily define his/her own aurora.

The chemical reactions and energy transfer processes resulting from electron deposition in the atmosphere are also described in the AARC manual.[2] Chemical kinetics mechanisms for NO, NO^+, and CO_2(4.3 μm) are currently being supplied as part of the SHARC-2 data base. The mechanisms include kinetic processes for ionization, electronic and vibrational excitation, recombination, chemical reactions, and formation of the secondary electron energy distribution. Upon exiting from the auroral module, aurorally enhanced populations are stored in an array for vibrationally excited species.

2.2.4 The Geometry Module

The GEOMETRY module in SHARC calculates a set of parameters which characterizes the line-of-sight (LOS) trajectory. There are three general categories of LOS's which are supported by SHARC:

- observer to a specified source location,
- observer to space, and
- limb viewing (space to space).

In addition to defining the LOS, the GEOMETRY module also calculates the column densities for ambient and vibrationally excited atmospheric species.

GEOMETRY is designed to give the user considerable flexibility in defining the LOS. It computes a uniform set of path quantities from one of many possible subsets of parameters specified by the user. For example, consider the parameters necessary to define the LOS for a path from an observer at Point A to a source at Point B. The LOS between these points can be specified by defining the altitude, longitude, and latitude for Point A, and either the altitude, longitude, and latitude for Point B, or the range between A and B and the zenith and azimuthal angles defined by the LOS direction. The full range of geometry inputs are discussed in Section 7.

2.2.5 The SPCRAD Module

SPCRAD computes the LOS spectral radiance using a finite-difference form of the radiative transfer equation. The LOS properties are specified in homogeneous segments where each segment corresponds to the LOS path through a particular atmospheric layer. A single-line equivalent width approximation based on the Voigt lineshape is used to determine the segment transmittances and radiances. This approach enables the spectral radiance to be calculated at a spectral resolution as high as 0.1 cm^{-1}, although the resolution in the current version of SHARC is set at 0.5 cm^{-1}. Since the radiation computation is explicitly based on the difference of the upper and lower state populations, it is equally valid in both the NLTE and LTE regimes. Line strengths and locations are taken from a modified line file generated from the AFGL HITRAN line atlas(5) and augmented with additional lines from various hot bands: currently the O_3 hot bands around 10 μm(6) and auroral NO and NO^+.(2) The major modification to the line parameter data base was to decompose the energy of the lower state into vibrational and rotational energies. This enables the line strengths to be scaled

separately for the rotational temperature and the NLTE vibrational population of the lower level.

There is a trade-off between speed and accuracy when the atmosphere is layered into many homogeneous layers. The LOS radiance calculation depends linearly on the number of layers. Currently the atmospheres used by SHARC are layered by 2 km from 50 to 150 km and by 10 km steps from 150 to 300 km. For a limb calculation at a tangent height of 50 km, up to 129 atmospheric layers are traversed by the LOS.

2.2.6 The OUTPUT Module

The OUTPUT module writes data and error statements to four separate data files. The files are the error file which is called "SHARC.ERR", the general output file, the spectral radiance file, transmittance file, and the 'population' files, which are named by the user.

"SHARC.ERR" will contain error and warning statements generated by a SHARC calculation. An error message is generated by a fatal problem in SHARC, and execution will stop after the error message is placed in the error file. A warning is not fatal to SHARC, but it may alert the user that only a partial calculation has been performed or that numerical difficulties have been encountered and fixed in some module of the code. The user should get in the habit of looking at the error file after every SHARC execution to insure that the full desired calculation was actually performed.

The output file contains a summary of the output from each module. There are three levels of output which can be obtained from each SHARC module. The level of output is selected through the interactive menu and can be defined independently for several of the SHARC subroutines or modules. The first level contains a minimum amount of information. For example, the minimum amount of information on the model atmosphere would be simply the model atmosphere name. The next level of output provides more

detailed information such as the number densities of the atmospheric species as a function of altitude, or the vibrational temperatures from the chemical kinetics module. Finally, the highest level of output provides intermediate results from within modules. This level of information may be necessary for "debugging" a problem encountered in SHARC, but is usually too detailed for day-to-day execution.

The spectral and transmission files contain the spectral radiance in $W/sr/cm^2/cm^{-1}$ as a function of frequency in cm^{-1} and the transmittance as a function of frequency in cm^{-1}. The resolution and frequency range is defined through the "SHARC.INP" file and/or the input module. Currently SHARC does not have a filter function routine. The data must be degraded by the application of a filter function after the SHARC calculation has been performed.

The population file saves the excited state populations and other necessary information so multiple SHARC calculations can be performed without re-calculating the populations each time. There are now two types of population files, ambient and auroral. The population files from each type of environment are saved in different format, so they can be used only with the proper environment type. The population for each layer in the model atmosphere will change only when either a new model atmosphere is used, day and night conditions change, a new solar zenith angle is defined, or auroral parameters are changed. By saving the populations, a user can build up a library of population files for the simulations of interest. Since the calculation of the NLTE populations requires roughly half of the calculation time required for a full SHARC run, considerable computational time can be saved by using population files.

2.3 Plotting Package

The plotting software is a separate package which can be used to plot the spectral output of a SHARC computation. The plotting program is a

general x-y plotting package. It is interactive and has two menus of options. The plotting package reads an input file which is a format-free list of x,y pairs without any header information. After the input file is read, plotting options can be changed through interactive menus. Default options are provided for convenience when plotting a SHARC output spectrum. The software can also be used for other plotting tasks. The plot and axis titles can contain superscripts, subscripts, as well as Greek and special characters. The program is written in Fortran 77. The program is designed to be as device independent as possible. It requires only standard Calcomp calls to initialize and terminate plotting, and a standard Calcomp call to move the pen.

3. SHARC INPUT FILES

3.1 INTERPRETER Files

The INTERPRETER reads the symbolic description of a chemical kinetics mechanism from an ASCII input file and writes the information describing the mechanism to a binary output file (the "linking" file) for subsequent use by the CHEMKIN module in SHARC. The input required by the INTERPRETER is the species name used in the mechanism and the mechanism itself. An example of the CO chemical kinetics mechanism input file currently used by SHARC is given in Table 1.

The information contained in the input file is given in an 80-column card format. All input to the INTERPRETER is format free. The INTERPRETER checks each input card for proper syntax and writes self-explanatory diagnostic messages to the output file if bad syntax is encountered. If any errors are encountered, the INTERPRETER does not create the linking file. Therefore, the input must be error free before SHARC can be executed.

The rules for creating the INTERPRETER input file have been described in detail in Reference (3). Subsections 3.1.1 and 3.1.2 have reproduced this input procedure as previously described. Some changes to the information expected in the SHARC INTERPRETER input file are incorporated in these sections.

TABLE 1. SHARC INTERPRETER CO KINETICS MECHANISM INPUT FILE.

```
CO SHARC CHEMICAL KINETICS MECHANISM
SPECIES
N2  O2  O  CO2  CO  H2O  NO  O3  H  OH
N2(0) N2(1) O2(0) O2(1)
CO(0) CO(1) CO(2)
END
REACTIONS
M + CO(1)  =  M + CO(0)                          9.90E-09   0.0   168.1    0.0
     N2/1.0/  O2/1.0/
O + CO(1)  =  O + CO(0)                          2.82E-09   0.0    75.4    0.0
M + CO(2)  =  M + CO(1)                          1.98E-08   0.0   168.1    0.0
     N2/1.0/  O2/1.0/
O + CO(2)  =  O + CO(1)                          2.82E-09   0.0    75.4    0.0
O + CO(2)  =  O + CO(0)                          2.82E-09   0.0    75.4    0.0
CO(0) + N2(1)  -  CO(1) + N2(0)                  6.98E-13   0.0    25.6    0.0
CO(1) + N2(0)  -  CO(0) + N2(1)                  6.98E-13   0.0    25.6  268.5
CO(1)  -  CO(0) + HV                              30.96     0.0     0.0    0.0
CO(2)  -  CO(1) + HV                              60.45     0.0     0.0    0.0
CO(2)  -  CO(0) + HV                               1.03     0.0     0.0    0.0
CO(0) + HV  -  CO(1)                                0.0     0.0     0.0    0.0
CO(0) + HV  -  CO(2)                                0.0     0.0     0.0    0.0
CO(1) + HV  -  CO(2)                                0.0     0.0     0.0    0.0
END
```

3.1.1 Species Cards

Each chemical species must be identified on a Species Card (or cards). Any set of up to 10 characters can be used as a species name, which must begin with a letter. Species names of more than 10 characters may be used by simply changing a parameter value and some related format statements in the INTERPRETER. The primary purpose of the Species Cards is to identify the atmospheric species, the vibrational states included in the chemical kinetics mechanism for the selected radiating species, and finally the order in which arrays of species information are referenced in SHARC.

The first Species Card must contain the word SPECIES starting in Column 1. It is then followed by any number of cards which identify the species. Species symbols may appear anywhere on the card, and those on the same card must be separated by blank spaces. After all the species have been given, the following card must contain the word END starting in Column 1. The rules for Species Cards are summarized in Table 2.

TABLE 2. SUMMARY OF THE RULES FOR SPECIES CARDS.

1. The first (last) species Card must contain the word SPECIES (END) starting in Column 1. All other columns on this card are ignored.

2. Species names are composed of up to 10-character symbols. The names cannot begin with the characters +, -, =, a parenthesis, or a number.

3. Each species must be declared only once.

4. Each species which subsequently appears in a reaction must be declared.

5. The species declarations may appear anywhere on the cards.

6. Any number of species declarations may appear on a card. More than one card may be used.

7. Species declarations which appear on the same card must be separated by at least one blank space.

8. A species declaration which begins on one card may not continue to the next card.

9. One species declaration may end in Column 80 of one card and the next declaration may begin in Column 1 of the next card.

3.1.2 Reaction Mechanism Description

The reaction mechanism may involve any number of chemical reactions and/or energy transfer processes involving the species named on the Species Cards. If more than 6 species appear in a given reaction, some dimension statements in the INTERPRETER must be changed. In the previous version of the INTERPRETER, the energy transfer/reactive processes were written explicitly in the forward and/or reverse directions. In the current version of the INTERPRETER, however, vibrational-to-translational energy transfer processes may be written in the forward direction (with reactants and products separated by delimiter "=" rather than "-"). SHARC-2 then computes the reverse rate constant using detailed balance. Vibrational-to-vibrational energy transfer processes must still be written explicitly in the forward and reverse direction. Processes may be three-body reactions with an arbitrary third body including the effects of enhanced third-body efficiencies, or may involve radiative relaxation and/or excitation (e.g., earthshine and/or sunshine).

The first Reaction Card must contain the word REACTIONS starting in Column 1. The following cards contain the reaction description together with the generalized Arrhenius/Schwartz-Slawsky-Herzfeld (SSH) rate coefficients. The reaction description is made up of Reaction Cards and perhaps Auxiliary Information Cards. The last card of the reaction description must contain the word END starting in Column 1.

3.1.2.1 Reaction Cards

Each Reaction Card is divided into two fields. The first field contains the symbolic description of the reaction while the second contains the Arrhenius/SSH rate coefficients. Both fields are format free, and blank spaces are ignored (except within a number or a species symbol). The reaction description, given in the first field, must be composed of the

species symbols, coefficients, delimiters, and special symbols as summarized below.

Species Symbols

Each species in a reaction is described with the unique sequence of characters exactly as they appear in the Species Cards.

Coefficients

Any species symbol may be preceded by an integer coefficient. The coefficient simply has the meaning that there are that many moles of the particular species present as either reactants or products; e.g., 2OH is equivalent to OH + OH (non-integer coefficients are not allowed).

Delimiters

\+ A plus sign is the delimiter between the reactant species and between the product species.

= An equality sign is the delimiter between the reactants and products for a reversible reaction.

\- A minus sign is the delimiter between the reactants and products for an irreversible reaction.

Special Symbols

M The symbol M stands for an arbitrary third body. Normally it would appear as both a reactant and a product. However, it has the identical meaning even if it appears only as a reactant or a product. In other words, an M anywhere in the reaction description indicates that a third body is participating in the reaction. In any reaction containing an M, species are specified to have third-body efficiencies, in which case the next card(s) must be Auxiliary Information cards (described below).

HV The symbol HV indicates that photon radiation ($h\nu$) is present as either a reactant or a product. If an HV appears in a reaction description, the wavelength of the radiation may be specified on an Auxiliary Information Card (described later).

E The symbol E is used to represent an electron. Electrons are treated just like any other species except that they are not composed of elements.

[An open bracket means that any following characters through the beginning of the numbers for the Arrhenius coefficients are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

A special case for reaction descriptions occurs if two or more species names are identical except for the last character in one of the names being a +, -, or = (e.g., NO, NO+). The INTERPRETER always seeks to find the longest possible species name between delimiters (+, -, =). Therefore, the species NO may not be followed directly by a + as a delimiter since this would be confused with the species NO+. To prevent this confusion, the species NO must be separated from the delimiter + by at least one blank space (e.g., the reaction NO+O+M = NO2+M must be written as NO +O+M = NO2+M). However, NO+ +E+M = NO +M may just as well be written as NO++M+E = NO +M as long as NO++ is not a species. There is no ambiguity in the convention, and the worst that can happen if the blank is not included before the delimiter is that an error message will be written from the INTERPRETER. The blank will have to be inserted by the user, but there is no possibility of having a reaction misinterpreted by the code and proceeding with an incorrect reaction.

The second field of the reaction card is used to define the Arrhenius/SSH rate coefficients A_i, β_i, C_i, and E_i. The rate constants are assumed to have the following functional form

$$k_i = A_i T^{\beta_i} \exp(-C_i/T^{1/3} - E_i/T) \qquad (5)$$

The four numbers must appear in order: the first number being A_i, the second being β_i, the third being C_i, and the fourth being E_i. At least one blank space must separate the first number and the last symbol in the reaction or the comment. The four numbers must be separated by at least one blank space; be stated in either integer, floating point, or E format

(e.g., 123 or 123.0 or 12.3E1) and have units associated with them. The default units for A_i are cgs (cm, sec, K, and molecules), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the SSH parameters and activation energies are $K^{1/3}$ and K, respectively.

Table 3 is a summary of the Reaction Card rules, and examples of some reaction cards are shown in Table 1.

TABLE 3. SUMMARY OF THE RULES FOR REACTION CARDS.

1. The first (last) Reaction Card must contain the word REACTIONS (END) starting in Column 1. All other columns on this card are ignored. (The END card would follow the last Auxiliary Information Card, if one was used for the last reaction).

2. The reaction description can begin anywhere on the card. All blank spaces, except those within species symbols and within coefficients, are ignored.

3. If some species names end with either the characters +, -, or =, and there are other species names which are identical to those except that they don't end in a +, -, or =, then in the reaction description the latter species names must be separated from +, -, or = delimiters by at least one blank space.

4. Each reaction description must use only one card and may not continue onto the next card.

5. Four numbers for the Arrhenius/SSH coefficients must appear on each Reaction Card, must occupy the last non-blank entries on the card, must be separated from the reaction description by at least one blank space, must be in the order (A_i, β_i, C_i, and E_i), and must be separated by at least one blank space. No blanks are allowed within the numbers themselves.

6. Comments are any characters following an open bracket and up to within one blank space of the first Arrhenius coefficient. The comments are written on on the output file along with the reaction description, but otherwise ignored within the code.

3.1.2.2 Auxiliary Information Cards

If a reaction contains an M as third body and/or it contains an HV to denote radiation, the card or cards following that reaction card may be Auxiliary Information Cards. These cards specify third-body efficiencies of certain species or specify radiation wavelength. Any species which acts as a third body must be declared as one of the species on the Species Cards.

The format of the card is a name (either a species name or the characters HV) followed by a number (either integer, floating point, or E format delimited by slashes(/). For enhanced third-body efficiencies, the name is the species name of the enhanced third body, and the number is its enhanced efficiency factor. For wavelength specification, the symbols HV are followed by the wavelength.

Any number of third-body efficiencies may be included, and each Auxiliary Information Card may contain one or more efficiency factors. If more than 6 species have are specified as third bodies in any one reaction, some dimensioning needs to be changed in the INTERPRETER. Also, the radiation wavelength may appear on a separate card, or it may be on the same card as a third-body efficiencies specification. Thus more than one Auxiliary Information Card may be used for any one reaction. Examples of auxiliary information are shown in Table 1. The above rules are summarized in Table 4.

TABLE 4. SUMMARY OF THE RULES FOR AUXILIARY INFORMATION CARDS.

1.	Auxiliary Information Cards may only follow Reaction Cards which contain an M or an HV.
2.	A species may have only one third-body efficiency associated with it in any one reaction.
3.	Only one radiation wavelength may be declared in a reaction.
4.	The order in which the enhanced third-body declarations are given is the order in which arrays of third-body information are referenced in the subroutine package. The order in which the radiation wavelength appears with respect to enhanced third-body information is unimportant.
5.	Third-body (or wavelength) information may appear anywhere on the card.
6.	Any number of third-body efficiencies may appear on a card. Thus more than one card may be used.
7.	Third-body declarations or radiation wavelength specifications which appear on the same card must be separated by at least one blank space.
8.	A third-body (or wavelength) declaration which begins on one card may not continue on to the next card.
9.	One declaration (third-body efficiency or wavelength) may end in column 80 of one card, and the next declaration may begin in Column 1 of the next card.
10.	Any blank spaces between the species symbol (or HV) and the first slash are ignored, and any blanks between the slashes and the efficiency factor (or wavelength) are also ignored. However, no blank spaces are allowed within the factor (or wavelength).

3.2 Molecular States Files

The molecular states files are designed to supply the following information to SHARC:

- Identification of the molecular radiator;
- Definition of the vibrational energies and degeneracies associated with the vibrational states included in the chemical kinetics mechanism;
- Definition of the vibrational transitions (i.e., molecular bands) which will be treated by NEMESIS and SPCRAD. Note that a transition may be considered by NEMESIS but not by SPCRAD; and
- Definition of an effective earthshine temperature for each transition considered by NEMESIS.

The molecular states file is written in ASCII format. The information is input in an 80 column format and is format free. The SHARC CO molecular states file is given in Table 5. As the structure of the molecular states file is described, the reader should refer back to Table 5 as an example of the file organization.

The first line in the states file identifies the radiating species (which must be the first entry on this line) being considered by SHARC. Any information contained on this line after the radiating species identification is treated only as a comment and is subsequently ignored by the code. The next line must contain the identifier ENERGIES starting in Column 1, and thus signals the start of the list of vibrational-state energies and degeneracies. This line is followed by any number of lines, each of which must contain three numbers to identify the particular vibrational state (using the standard AFGL notation), the energy of that state (in cm^{-1}), and the degeneracy of that state, respectively. The three numbers must be separated by at least one blank, and may be integer, floating point, or exponential format. After all the vibrational states have been listed, the next line must contain the word END beginning in Column 1.

TABLE 5. SHARC CO MOLECULAR STATES INPUT FILE.

```
CO VIBRATIONAL STATES AND TRANSITIONS
ENERGIES AND DEGENERACIES
 0     0.000      1
 1  2143.272      1
 2  4260.063      1
END
TRANSITIONS
 1-0      230.0      1
 2-0      280.0      1
 2-1      280.0      1
END
```

The next section of the molecular states file lists the vibrational transitions information. The first line following the END card must contain the word TRANSITIONS starting in Column 1. This line is followed by as many lines as necessary to identify: each vibrational transition considered by NEMESIS, the effective earthshine temperature (in K) for the transition, and whether or not to compute the radiance along the observer LOS for the transition. The vibrational transition is listed as "U-L" where "U" denotes the upper state and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. It is important to note that a transition in the molecular states file must have the corresponding radiative relaxation and excitation processes listed in the chemical kinetics mechanism (compare Tables 1 and 5). The LOS radiance option is defined as follows:

- 0 - Radiance is <u>not</u> computed for this transition,
- 1 - Radiance is computed for this transition.

Although the radiance may not be computed for a particular transition, it may be important to include the transition in the states file for the

NEMESIS calculation. The vibrational transition, effective earthshine temperature, and LOS radiance option must be separated by at least one blank. After all the vibrational transitions information has been given, a line containing the word END beginning in Column 1 must follow.

3.3 Molecular Bands Files

The molecular bands files are used to input line strength information necessary for the ambient population module. Bands files are not used in the auroral calculations. The bands information is used to obtain the altitude-dependent earthshine and sunshine excitation rates, and to calculate the enhancement of molecular excited-state populations due to radiative trapping and atmospheric emission.

Although the ambient population module could directly use the modified HITRAN line compilation, this would be extremely time consuming due to the large number of lines. It is much more efficient to discretize the line strength distribution. Finite width bins are chosen in which a single average line is determined and a degeneracy equal to the actual number of lines from the exact distribution is assigned to the average line. In the limit of infinitesimal width bins the exact line strength distribution is recovered. For reasonable choices of bin widths (presently three bins per order of magnitude), the number of lines that need be considered can be reduced by several orders of magnitude without significant loss of computational accuracy.

The molecular bands file indicates the vibrational transition along with the number of lines in a bin, and the average strength in the bin at the specified temperature. This information suffices to completely characterize the discretized line strength distribution at each temperature. The file is written in ASCII format assuming an 80 column line and is format free. The SHARC CO molecular bands file is given in Table 6. Again, the reader should refer back to Table 6 as an example of the file organization.

The first line in the bands file identifies the molecular species (which must be the first entry on this line) for which the file has been created. The information contained on this line after the species identification is treated only as a comment and is ignored by the code. The molecular species is checked against the radiating species identified in the molecular states file to ensure a consistent set of files is being used. The second line contains the vibrational transition which is then followed by a list of the line strength parameters. As in the molecular states file, the vibrational transition is listed as "U-L" where "U" denotes the upper state, and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. <u>Each transition listed in the molecular states file must have a corresponding entry in the molecular bands file.</u> The next line notes the number of temperatures and the temperatures at which the strength distribution was calculated. The following lines describe the line strength distribution. Each line contains the number of lines in that energy bin and the average line strength at each T_n. The entries must be in the following order: (1) the number of lines in the bin, (2) the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_1, (3) the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_2 continuing up to the nth temperature. After all the line strength bins have been listed for the particular transition, the next line must contain the word END beginning in Column 1.

TABLE 6. SHARC CO MOLECULAR BANDS INPUT FILE.

```
CO      BAND TRANSITIONS FOR ISOTOPE NUMBER 1
        1-       0    G      SBAR       SBAR       SBAR       SBAR       SBAR
                      5      200.       250.       300.       500.      1000.
                     19 0.407E-18  0.376E-18  0.346E-18  0.257E-18  0.146E-18
                      8 0.179E-18  0.195E-18  0.203E-18  0.199E-18  0.142E-18
                      5 0.845E-19  0.127E-18  0.163E-18  0.229E-18  0.209E-18
                      3 0.392E-19  0.704E-19  0.101E-18  0.178E-18  0.192E-18
                      4 0.180E-19  0.386E-19  0.623E-19  0.140E-18  0.181E-18
                      2 0.838E-20  0.214E-19  0.386E-19  0.109E-18  0.166E-18
                      4 0.387E-20  0.116E-19  0.234E-19  0.823E-19  0.149E-18
                      2 0.156E-20  0.571E-20  0.132E-19  0.601E-19  0.132E-18
                      2 0.837E-21  0.351E-20  0.883E-20  0.481E-19  0.120E-18
                      7 0.228E-21  0.122E-20  0.363E-20  0.285E-19  0.965E-19
END
        2-       0    G      SBAR       SBAR       SBAR       SBAR       SBAR
                      5      200.       250.       300.       500.      1000.
                     19 0.312E-20  0.288E-20  0.266E-20  0.198E-20  0.117E-20
                      9 0.131E-20  0.146E-20  0.155E-20  0.158E-20  0.121E-20
                      4 0.587E-21  0.906E-21  0.117E-20  0.170E-20  0.166E-20
                      3 0.294E-21  0.528E-21  0.756E-21  0.134E-20  0.151E-20
                      4 0.139E-21  0.299E-21  0.481E-21  0.108E-20  0.146E-20
                      3 0.579E-22  0.152E-21  0.281E-21  0.831E-21  0.138E-20
                      2 0.288E-22  0.872E-22  0.177E-21  0.631E-21  0.121E-20
                      3 0.142E-22  0.495E-22  0.110E-21  0.475E-21  0.104E-20
                      2 0.652E-23  0.273E-22  0.687E-22  0.375E-21  0.981E-21
                      7 0.179E-23  0.955E-23  0.285E-22  0.225E-21  0.798E-21
END
        2-       1    G      SBAR       SBAR       SBAR       SBAR       SBAR
                      5      200.       250.       300.       500.      1000.
                     19 0.808E-18  0.745E-18  0.685E-18  0.508E-18  0.288E-18
                      8 0.326E-18  0.380E-18  0.413E-18  0.434E-18  0.323E-18
                      4 0.156E-18  0.239E-18  0.308E-18  0.441E-18  0.406E-18
                      3 0.802E-19  0.143E-18  0.203E-18  0.356E-18  0.380E-18
                      5 0.395E-19  0.711E-19  0.108E-18  0.229E-18  0.289E-18
                      3 0.153E-19  0.396E-19  0.726E-19  0.210E-18  0.329E-18
                      3 0.714E-20  0.216E-19  0.439E-19  0.157E-18  0.286E-18
END
```

3.4 Modified HITRAN Line File

The augmented HITRAN[5] line file used by SHARC includes line parameters for CO, OH, CO_2, H_2O, O_3, NO+, and NO. There are a total of 155,000 lines in the file, although the bands currently supported by SHARC will use 91,000 of the lines. The other lines are for transitions which will be supported in future versions of SHARC. The lines in the file have been modified to speed up the LOS spectral radiance calculation. The first modification was to separate the total energy of the lower state, E", into vibrational, E_V, and rotational, E_R, components. SHARC requires the separate E_V and E_R to properly scale the line strength since there are different vibrational and rotational temperatures. Computational time is saved by storing E" and E_R rather than re-calculating them in the spectral radiance module.

The standard HITRAN line strengths have also been modified. The temperature-dependent scaling factors evaluated at the reference temperature, $T_s = 296$ K, have been removed from the strengths. This modification speeds up the spectral radiance calculation by eliminating the calculations which depend on T_s. Although the CPU savings realized by removing T_s is fairly small per line, a typical calculation uses thousands of lines and, therefore, the total savings can be significant. The line strength, SR, stored in the database is given by:

$$SR = S(T_s)\ Q_v(T_s)\ Q_r(T_s)\ Q_e(T_s)\ \exp(C_2 \frac{E''}{T_s})\ [1 - \exp(-C_2 \frac{W_o}{T_s})]^{-1} \qquad (7)$$

where $S(T_s)$ is the standard HITRAN line strength, W_o is the transition wavenumber, Q_v, Q_r and Q_e are the vibrational, rotational and electronic partition functions, respectively.

The following database parameters are used in the spectral radiance module of SHARC:

MOL - AFGL molecular species identification label

ISO - AFGL molecular species isotope identification label

W_o - transition frequency (cm^{-1})

SR - modified line strength (cm^{-1}/molecule/cm^{-2})

GAM - Lorentz halfwidth (cm^{-1})

E" - total energy of lower state (cm^{-1})

E_R - rotational energy of lower state (cm^{-1})

IUP - upper state vibrational label

ILOW - lower state vibrational label.

In addition to the above parameters, there are a few parameters in the database that are not currently used by SHARC but are included to support future extensions. These include a self-broadening halfwidth, a coefficient of temperature dependence of air-broadened halfwidth, and upper and lower state local quanta indices. An example of the database is given in Table 7; we have included only the parameters currently used by SHARC. This part of the line file includes lines for H_2O (MOL=1), CO_2 (MOL=2), and NO (MOL=8).

The line file used by SHARC is written in binary format. Using a binary representation of the file saves storage space and makes the reading time shorter than if the file was stored in an ASCII format. The file is provided on the SHARC computer tape in an ASCII format along with a program which converts the file to binary.

TABLE 7. PART OF SHARC LINE PARAMETER DATABASE.

MOL	ISO	W_O	SR	GAM	E"	E_R	IUP	ILOW
1	1	1950.4490	.432E-16	.0907	2000.8660	406.1160	4	2
2	1	1950.6992	.727E-21	.0727	197.4163	197.4163	6	1
2	1	1950.8227	.212E-19	.0646	1308.6709	641.2909	11	2
8	1	1950.8421	.149E-18	.0500	4514.8540	790.6841	4	13
8	1	1950.8650	.103E-15	.0490	1189.3781	1189.3781	2	1
8	1	1950.8710	.103E-15	.0490	1189.4390	1189.4390	2	1
8	1	1950.9238	.248E-19	.0610	3737.2720	13.1021	4	13
2	1	1950.9821	.191E-19	.0649	1276.4469	609.0669	11	2
1	1	1951.1300	.113E-17	.0620	447.2520	447.2520	2	1
2	1	1951.1772	.199E-20	.0892	1390.5258	2.3407	19	5
2	1	1951.1910	.358E-20	.0876	1395.9884	7.8033	19	5
2	1	1951.2126	.518E-20	.0860	1404.5724	16.3873	19	5
2	1	1951.2421	.677E-20	.0843	1416.2777	28.0927	19	5
2	1	1951.2794	.835E-20	.0826	1431.1040	42.9189	19	5
2	1	1951.3244	.996E-20	.0810	1449.0513	60.8662	19	5
3	1	1951.3430	.679E-18	.0638	652.3090	652.3090	14	1
2	1	1951.3772	.115E-19	.0793	1470.1191	81.9341	19	5
1	1	1951.4230	.137E-16	.0820	1907.4520	312.7020	4	2
2	1	1951.4375	.131E-19	.0777	1494.3074	106.1223	19	5
2	1	1951.5055	.147E-19	.0761	1521.6157	133.4307	19	5
2	1	1951.5810	.163E-19	.0747	1552.0435	163.8584	19	5
2	1	1951.6639	.179E-19	.0733	1585.5906	197.4055	19	5
2	1	1951.7541	.195E-19	.0721	1622.2563	234.0713	19	5
8	1	1951.7804	.151E-18	.0500	4588.4712	864.3013	4	13
8	1	1951.8076	.551E-19	.0570	5738.5718	194.4468	5	14
2	1	1951.8515	.211E-19	.0710	1662.0403	273.8552	19	5
2	1	1951.9560	.227E-19	.0699	1704.9419	316.7568	19	5

3.5 Model Atmosphere Files

The atmospheric models supplied with SHARC are based on a fairing of the AFGL standard profiles(7) and the HAIRM(6) atmospheric models. There are currently daytime and nighttime models for 1976 standard atmosphere and subarctic summer. These models include temperature and number densities for N_2, O_2, O, OH, CO_2, H_2O, NO, H, O_3, and CO as a function of altitude. The profiles are layered into 50 homogeneous layers (66 layer boundaries)

defined in 2 km increments from 50 to 150 km and in 10 km increments from 150 to 300 km.

The model atmosphere file is contained in an 80 column, format free ASCII file. The input file is checked for proper syntax and self-explanatory diagnostic messages are written to the SHARC error file if unacceptable syntax is encountered.

The user can define a new atmosphere file by following a set of simple rules. A SHARC atmospheric file is structured as a series of input parameter identification cards followed by the actual input values (at least one) and an END card that denotes the end of the parameter input.

As an example, the daytime 1976 Standard Atmosphere Model input file provided with SHARC is shown in Table 8. As the various input parameters are described, it should help the user to refer back to Table 8.

TABLE 8. CURRENT SHARC 1976 STANDARD MODEL ATMOSPHERE INPUT FILE.

```
ATMOSPHERE NAME
DAY76.DAT
END
NUMBER OF LAYERS
 66
END
DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE
  DAY  1000.
END
SPECIES
N2 O2 O CO2 CO H2O NO O3 H OH
END
ALTITUDES
50 52 54 56 58
60 62 64 66 68
70 72 74 76 78
80 82 84 86 88
90 92 94 96 98
100 102 104 106 108
110 112 114 116 118
120 122 124 126 128
130 132 134 136 138
140 142 144 146 148
```

```
150 160 170 180 190
200 210 220 230 240
250 260 270 280 290
300
END
TEMPERATURES
      270.65      269.0       263.5       258.0       252.5
   2.4706E+02 2.4157E+02 2.3607E+02 2.3058E+02 2.2509E+02
   2.1959E+02 2.1426E+02 2.1035E+02 2.0643E+02 2.0252E+02
   1.9861E+02 1.9470E+02 1.9078E+02 1.8687E+02 1.8687E+02
   1.8687E+02 1.8698E+02 1.8774E+02 1.8931E+02 1.9172E+02
   1.9508E+02 1.9953E+02 2.0531E+02 2.1289E+02 2.2329E+02
   2.4000E+02 2.6400E+02 2.8800E+02 3.1200E+02 3.3600E+02
   3.6000E+02 3.8355E+02 4.0622E+02 4.2804E+02 4.4904E+02
   4.6927E+02 4.8838E+02 5.0748E+02 5.2519E+02 5.4290E+02
   5.5932E+02 5.7573E+02 5.9095E+02 6.0617E+02 6.2028E+02
   6.3439E+02 6.9629E+02 7.4757E+02 7.9007E+02 8.2531E+02
   8.5456E+02 8.7679E+02 8.9901E+02 9.0739E+02 9.1578E+02
   9.3338E+02 9.5099E+02 9.5724E+02 9.6350E+02 9.6976E+02
   9.7601E+02
END
N2 DENSITIES
    1.67E+16    1.32E+16    1.04E+16    8.17E+15    6.40E+15
   5.0401E+15 3.9179E+15 3.0285E+15 2.3272E+15 1.7774E+15
   1.3487E+15 1.0158E+15 7.5547E+14 5.5885E+14 4.1110E+14
   3.0067E+14 2.1[illegible]59E+14 1.5792E+14 1.1335E+14 7.915E+13
   5.547E+13  3.8860E+13 2.7150E+13 1.8940E+13 1.3200E+13
   9.2100E+12 6.5080E+12 4.6090E+12 3.2730E+12 2.3270E+12
   1.6410E+12 1.1580E+12 8.4220E+11 6.2850E+11 4.7940E+11
   3.7260E+11 2.9470E+11 2.3680E+11 1.9300E+11 1.5920E+11
   1.3260E+11 1.1160E+11 9.4600E+10 8.0800E+10 6.9470E+10
   6.0090E+10 5.2250E+10 4.5650E+10 4.0070E+10 3.5310E+10
   3.1240E+10 1.7740E+10 1.0700E+10 6.7400E+09 4.3850E+09
   2.9250E+09 1.9890E+09 1.3730E+09 9.6000E+08 6.7780E+08
   4.8260E+08 3.4590E+08 2.4940E+08 1.8060E+08 1.3140E+08
   9.5930E+07
END
O2 DENSITIES
     4.46E+15    3.52E+15    2.78E+15    2.19E+15    1.71E+15
   1.3521E+15 1.0510E+15 8.1245E+14 6.2433E+14 4.7682E+14
   3.6181E+14 2.7251E+14 2.0267E+14 1.4992E+14 1.1029E+14
   8.0661E+13 5.8641E+13 4.2366E+13 3.0310E+13 2.1200E+13
   1.4790E+13 1.0270E+13 7.0600E+12 4.8010E+12 3.2300E+12
   2.1510E+12 1.4300E+12 9.4340E+11 6.1890E+11 4.0450E+11
   2.6210E+11 1.7060E+11 1.1560E+11 8.1200E+10 5.8920E+10
   4.3950E+10 3.3600E+10 2.6250E+10 2.0870E+10 1.6830E+10
   1.3750E+10 1.1340E+10 9.4440E+09 7.9270E+09 6.7020E+09
   5.7020E+09 4.8810E+09 4.1990E+09 3.6310E+09 3.1530E+09
   2.7500E+09 1.4600E+09 8.2770E+08 4.9210E+08 3.0310E+08
```

```
  1.9180E+08 1.2390E+08 8.1450E+07 5.4250E+07 3.6530E+07
  2.4820E+07 1.7000E+07 1.1710E+07 8.1100E+06 5.6430E+06
  3.9420E+06
END
O DENSITIES
    8.00E+09    8.66E+09    9.41E+09    1.02E+10    1.11E+10
  1.2000E+10 1.3291E+10 1.4720E+10 1.6304E+10 1.8058E+10
  2.0000E+10 2.4915E+10 3.1037E+10 3.8664E+10 4.8164E+10
  6.0000E+10 6.7650E+10 7.6275E+10 8.6000E+10 1.5100E+11
  2.4430E+11 3.4340E+11 4.1590E+11 4.4710E+11 4.4760E+11
  4.2980E+11 4.0070E+11 3.6190E+11 3.1880E+11 2.7480E+11
  2.3030E+11 1.8890E+11 1.5650E+11 1.3050E+11 1.0960E+11
  9.2750E+10 7.9250E+10 6.8400E+10 5.9560E+10 5.2290E+10
  4.6250E+10 4.1180E+10 3.6880E+10 3.3200E+10 3.0040E+10
  2.7290E+10 2.4890E+10 2.2780E+10 2.0920E+10 1.9270E+10
  1.7800E+10 1.2380E+10 8.9960E+09 6.7470E+09 5.1810E+09
  4.0500E+09 3.2110E+09 2.5730E+09 2.0810E+09 1.6950E+09
  1.3880E+09 1.1430E+09 9.4470E+08 7.8340E+08 6.5160E+08
  5.4330E+08
END
CO2 DENSITIES
    7.05E+12    5.56E+12    4.39E+12    3.45E+12    2.71E+12
  2.0268E+12 1.5755E+12 1.2178E+12 9.3586E+11 7.1474E+11
  5.4235E+11 4.0849E+11 3.0380E+11 2.2473E+11 1.6532E+11
  1.2091E+11 8.7901E+10 6.3505E+10 4.5582E+10 3.1936E+10
  2.2380E+10 1.5[illegible]79E+10 1.0958E+10 7.6444E+09 5.3303E+09
  3.7193E+09 2.5999E+09 1.8222E+09 1.2809E+09 9.0199E+08
  6.3096E+08 3.8519E+08 2.4553E+08 1.6228E+08 1.1063E+08
  7.7452E+07 5.5552E+07 4.0724E+07 3.0420E+07 2.3095E+07
  1.7785E+07 1.3878E+07 1.0934E+07 8.7128E+06 6.9961E+06
  5.6699E+06 4.6236E+06 3.7995E+06 3.1382E+06 2.6089E+06
  2.1781E+06 9.4394E+05 4.4431E+05 2.2195E+05 1.1589E+05
  6.2601E+04 3.4781E+04 1.9643E+04 1.1394E+04 6.6526E+03
  3.8811E+03 2.2906E+03 1.3793E+03 8.3449E+02 5.0729E+02
  3.0983E+02
END
H2O DENSITIES
    1.12E+11     8.73E+10     6.82E+10     5.26E+10     4.10E+10
    3.35E+10     2.60E+10     2.04E+10     1.51E+10     1.09E+10
    7.92E+09     5.75E+09     3.87E+09     2.61E+09     1.68E+09
    1.06E+09     6.58E+08     3.59E+08     2.03E+08     1.14E+08
    6.14E+07     3.44E+07     1.84E+07     1.05E+07     6.34E+06
    3.77E+06     2.34E+06     1.[illegible]E+06     8.42E+05     4.81E+05
   256000.      137000.       66900.       33600.       26000.
    20400.       16300.       13300.       10900.        9130.
     7710.        6570.        5630.        4880.        4250.
     3720.        3280.        2900.        2580.        2310.
     2070.        1260.         822.         560.         395.
      287.         213.         161.         124.          96.
```

```
       76.          60.          48.          39.          32.
       26.
END
NO DENSITIES
  2.20E+08    1.72E+08    1.34E+08    1.06E+08    8.28E+07
 6.4902E+07 5.0625E+07 3.9488E+07 3.1146E+07 2.4842E+07
 1.9814E+07 1.6964E+07 1.4523E+07 1.2734E+07 1.1436E+07
 1.0269E+07 1.0927E+07 1.1627E+07 1.5138E+07 1.9711E+07
 2.5663E+07 3.2704E+07 4.1846E+07 5.2882E+07 6.1872E+07
 7.2242E+07 7.5363E+07 7.7797E+07 7.7797E+07 7.8731E+07
 7.8731E+07 7.5313E+07 7.3370E+07 7.0153E+07   6.60E+07
   6.15E+07   5.60E+07 4.9804E+07 4.3494E+07 3.7780E+07
 3.2572E+07 2.7847E+07 2.4532E+07 2.1422E+07 1.8715E+07
 1.6325E+07 1.4088E+07 1.2350E+07 1.0999E+07 9.5536E+06
 8.1918E+06 4.1238E+06 2.1095E+06 1.2207E+06 804494.187
 530173.87  349392.59  230255.04  151741.56  100000.0
 65641.976  43088.691  28284.269  18566.353  12187.323
 8000.0
END
CO DENSITIES
    9.83E+08    9.13E+08    8.29E+08    7.79E+08    7.44E+08
   9.000E+08   1.050E+09   1.250E+09   1.430E+09   1.550E+09
   1.680E+09   1.840E+09   1.920E+09   1.960E+09   1.930E+09
   1.830E+09   1.680E+09   1.510E+09   1.280E+09   1.000E+09
   7.810E+08   6.720E+08   5.100E+08   4.000E+08   3.000E+08
   2.230E+08   1.630E+08   1.200E+08   8.760E+07   6.440E+07
   4.700E+07   3.590E+07   2.800E+07   2.250E+07   1.840E+07
   1.530E+07   1.260E+07   1.060E+07   9.040E+06   7.750E+06
   6.830E+06   5.810E+06   5.000E+06   4.320E+06   3.760E+06
   3.300E+06   2.910E+06   2.570E+06   2.290E+06   2.050E+06
   1.850E+06   1.090E+06   7.000E+05   4.700E+05   2.980E+05
   1.950E+05   1.300E+05   9.070E+04   6.570E+04   4.890E+04
   3.800E+04   3.020E+04   2.420E+04   1.940E+04   1.580E+04
   1.290E+04
END
O3 DENSITIES
   6.64E+10    3.84E+10    2.55E+10    1.61E+10    1.12E+10
   7.30E+09    4.80E+09    3.10E+09    1.80E+09    8.70E+08
   3.80E+08    1.70E+08    8.20E+07    4.20E+07    3.00E+07
   4.00E+07    7.30E+07    9.00E+07    8.60E+07    6.80E+07
   4.90E+07    3.40E+07    2.00E+07    1.20E+07    6.10E+06
   3.00E+06    1.40E+06    6.60E+05    2.90E+05    1.30E+05
 51400.      18900.       7650.       3330.       1560.
   767.        442.0       254.0       146.7        84.7
    49.0        33.         23.         16.         10.6
     7.2         5.4         4.0         3.0         2.2
     1.66         .58         .20    7.100E-02   2.500E-02
```

```
    8.60E-03   4.700E-03   2.600E-03   1.400E-03   7.600E-04
    4.80E-04   2.400E-04   1.400E-04   8.100E-05   4.700E-05
    2.70E-05
END
H DENSITIES
    3.28E+05    5.28E+05    7.83E+05    1.12E+06    1.72E+06
    2.66E+06    4.12E+06    6.24E+06    9.91E+06    1.55E+07
    2.30E+07    3.26E+07    4.05E+07    4.37E+07    3.97E+07
    3.23E+07    2.31E+07    1.69E+07    1.61E+07    2.98E+07
    5.60E+07    6.54E+07    5.95E+07    4.84E+07    3.78E+07
    2.87E+07    2.18E+07    1.64E+07    1.26E+07    9.73E+06
    7.56E+06    6.41E+06    5.44E+06    4.46E+06    3.48E+06
    2.51E+06    2.14E+06    1.82E+06    1.51E+06    1.20E+06
    9.12E+05    8.08E+05    7.03E+05    5.98E+05    4.93E+05
    3.88E+05    3.37E+05    2.92E+05    2.47E+05    2.02E+05
    1.60E+05    7.13E+04    3.45E+04    1.71E+04    8.00E+03
    4.08E+03    2.02E+03    1.05E+03    6.10E+02    3.15E+02
    1.74E+02    1.03E+02    5.81E+01    3.19E+01    1.78E+01
    9.73E+00
END
OH DENSITIES
     1.44E+07     1.32E+07     1.19E+07     1.16E+07     1.14E+07
    1.131E+07    1.183E+07    1.238E+07    1.261E+07    1.250E+07
    1.239E+07    1.107E+07    9.890E+06    8.015E+06    5.891E+06
    4.330E+06    2.451E+06    1.387E+06    6.276E+05    2.269E+05
    8.206E+04    [illegible].079E+04    1.155E+04    4.216E+03    1.497E+03
    5.660E+02    2.620E+02    1.420E+02    8.680E+01    5.750E+01
    4.030E+01    3.000E+01    2.250E+01    1.730E+01    1.370E+01
    1.030E+01    8.250E+00    6.720E+00    5.590E+00    4.730E+00
    3.980E+00    3.400E+00    2.900E+00    2.520E+00    2.180E+00
    1.914E+00    1.684E+00    1.490E+00    1.322E+00    1.182E+00
    1.058E+00    6.440E-01    4.160E-01    2.820E-01    1.990E-01
    1.444E-01    1.078E-01    8.100E-02    6.240E-02    4.860E-02
    3.800E-02    3.020E-02    2.420E-02    1.942E-02    1.578E-02
    1.282E-02
END
```

The following input parameter identification cards must be contained in the user-defined atmospheric model file in the order listed:

- ATMOSPHERE NAME Card
- NUMBER OF LAYER BOUNDARIES Card
- DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE Card
- SPECIES Card
- ALTITUDES Card

- TEMPERATURES Card
- SPECIES DENSITIES Card.

Each input parameter identification card must start in Column 1. After the appropriate data corresponding to the identification card has been entered into the file, the next line must contain the word END beginning in Column 1. The information required after each parameter identification card is detailed below.

The line following the ATMOSPHERE NAME card must contain the alphanumeric name of the atmospheric file being used. Up to 32 non-blank characters are allowed. After the END card (and following the NUMBER OF LAYER BOUNDARIES card), the number of layer boundary points should be entered. There must be at least two layer boundaries, and the current maximum is 61 boundaries. Next the DAY-NIGHT parameter and the EXOATMOSPHERIC TEMPERATURE should be defined exactly in the order stated and separated by at least a blank space. The DAY-NIGHT parameter is entered as either DAY or NIGHT. For a user-defined atmosphere the DAY-NIGHT parameter must be present, but it is not actually used by SHARC. After the SPECIES card, a list of atmospheric species for which number densities are given is input. This list of species must include all molecular species desired in the model atmosphere. The same rules apply to entering the atmospheric species as those given for the INTERPRETER (see Subsection 3.1.1). Also, each species listed in the atmosphere file must be listed as a species in the interpreter file. The next input considered is the altitudes of the layer boundaries. Any number of lines may be entered to define the layer altitudes. The layers must be entered in ascending order. The input units are km and are converted to cm internally. Next the kinetic temperatures and species number densities are entered in such a way as to correspond to the layer boundary altitudes. The number of entries for the temperatures and each species number densities must equal the value of the parameter entered for the number of layer boundaries. The temperatures are input in degrees Kelvin and the

number densities are input in molecules/cm^3. After the line containing the END card for the TEMPERATURE data, a card with one of the valid atmospheric species names (followed by a blank and the word DENSITIES) indicates the beginning of the atmospheric number densities input for this species, see Table 8 for clarification. Again, this data is followed by the word END beginning in Column 1. The procedure for the atmospheric species is continued until number densities have been defined for all atmospheric species listed in the SPECIES section of the file.

4. RUNNING SHARC

4.1 Overview

This section is intended as a ready reference for the user who has some familiarity with running SHARC-2, but may want a quick tutorial for the execution procedure. In addition to providing somewhat brief instructions taking the user from the input files through to a plot of spectral radiance, file names used by the INTERPRETER, SHARC, and the PLOTTING PACKAGE are also presented. Of course, for detailed instructions concerning the creation of input files or definition of input variables, the user should refer to the appropriate sections of this report.

Prior to running SHARC, the "linking" files must be created for each molecular radiator. This is accomplished by running the INTERPRETER once for each radiator. The INTERPRETER expects an ASCII input file named INTERP.INP, which contains the chemical kinetics mechanism for producing vibrationally excited states for the selected radiator. The structure for this input file is discussed in some detail in Section 3.1. After executing the INTERPRETER, two output files are created: INTERP.OUT and INTERP.LNK. The file INTERP.OUT is an ASCII file and contains information from the input file. The user should check this file to ensure that the INTERPRETER was successfully executed. Any error messages created during program execution will be written to this file. The file INTERP.LNK is a binary file (i.e., the "linking" file) which contains the chemical kinetics information required by SHARC. This file is only created if no errors were encountered during the INTERPRETER execution.

There are eight chemical kinetics mechanism input files which are currently supplied with SHARC for CO, NO, H_2O, O_3 and three isotopes of CO_2. There are also auroral kinetic files for the primary isotope of CO_2, NO^+ and NO. The input file names are summarized in Table 9. In order to create a "linking" file for one of the radiators, say CO, one would proceed

as follows: (1) copy the file COKIN.DAT to INTERP.INP, (2) execute the INTERPRETER, (3) rename INTERP.OUT to COOUT.DAT, and (4) rename INTERP.LNK to COLINK.DAT. The file COLINK.DAT would then be used as the "linking" file for SHARC. This procedure should be carried out for each molecular radiator.

TABLE 9. SUMMARY OF THE FILES USED BY THE INTERPRETER.

INPUT	OUTPUT	LINKING
H2OKIN.DAT	H2OOUT.DAT	H2OLINK.DAT
CO21KIN.DAT	CO21OUT.DAT	CO21LINK.DAT
CO22KIN.DAT	CO22OUT.DAT	CO22LINK.DAT
CO23KIN.DAT	CO23OUT.DAT	CO23LINK.DAT
O3KIN.DAT	O3OUT.DAT	O3LINK.DAT
COKIN.DAT	COOUT.DAT	COLINK.DAT
NOKIN.DAT	NOOUT.DAT	NOLINK.DAT
ACO2KIN.DAT	ACO2OUT.DAT	ACO2LINK.DAT
ANOKIN.DAT	ANOOUT.DAT	ANOLINK.DAT
ANOPKIN.DAT	ANOPOUT.DAT	ANOPLINK.DAT

To execute SHARC the user must first prepare several input files. Many of these files require no modification by the user unless the user desires to change and/or supplement the AFGL database provided with SHARC. The SHARC input and output files are summarized in Table 10. These files include:

- 10 Linking files (one for each molecular emitter),
- 10 States files (one for each molecular emitter),
- 7 Bands files (one for each molecular emitter, none required for auroral species),
- 1 Model atmosphere profile file (four are provided),
- SHARC HITRAN file (binary version), and
- SHARC input file (SHARC.INP).

TABLE 10. SUMMARY OF THE FILES USED BY SHARC.

LINKING	STATES	BANDS	INPUT	OUTPUT
COLINK.DAT	COSTAT.DAT	COBAND.DAT	SHARC.INP	SHARC.ERR
NOLINK.DAT	NOSTAT.DAT	NOBAND.DAT	SHARC.LIN	SHARC.OUT*
CO21LINK.DAT	CO21STAT.DAT	CO21BAND.DAT	DAY76.DAT%	SHARC.SPC*
CO22LINK.DAT	CO22STAT.DAT	CO22BAND.DAT		SHARC.TRN*
CO23LINK.DAT	CO23STAT.DAT	CO23BAND.DAT		POPNEW.DAT*
H2OLINK.DAT	H2OSTAT.DAT	H2OBAND.DAT		
O3LINK.DAT	O3STAT.DAT	O3BAND.DAT		
ACO2LINK.DAT	ACO2STAT.DAT			
ANOLINK.DAT	ANOSTAT.DAT			
ANOPLINK.DAT	ANOPSTAT.DAT			

% This is one of the 4 model atmosphere files supplied.

* User-supplied name.

These files have been described in detail in Sections 3 and 4 of this manual. The Linking files are generated by running the INTERPRETER as described above. The states, bands, and model atmosphere files are provided on the SHARC computer tape, and require no modification. The binary SHARC HITRAN file is generated from an ASCII file provided on the SHARC computer tape. Forming this binary file and compiling/linking SHARC are described in Appendix A. Finally the SHARC input file, SHARC.INP, must be available to SHARC, or a new SHARC.INP will be created. The input module and the SHARC.INP files are described in detail in Sections 4.2 - 4.4.

Once the user has all of the above files prepared, SHARC can be executed. SHARC can run in either an interactive or batch/background mode of operation. The interactive mode is useful in setting up new calculation scenarios, since the interactive input module can walk the user through the necessary input variables. For more experienced users, SHARC can be executed by circumventing the input module and making all changes to the SHARC.INP file with an editor.

The input module of SHARC is based on a menu-query system derived from the AFGL Auroral Atmospheric Radiance Code.[2] In general, typing a 0 will take the user up a level in the menu system, while typing a number greater than 0 will allow the user to input new information or enter a submenu. When a submenu is entered the current values for input variables are displayed to the user. This allows the user to scan the current input parameter values and decide if anything needs to be changed. There is a sample interactive session in Section 4.2.

After a successful SHARC calculation there will be between five and seven new ASCII output files. These files are:

- Error file (described in Section 5.1),
- General output file (described in Section 5.2),
- One to three Population files (described in Section 5.3),
- Spectral radiance file (described in Section 5.4), and
- Transmittance file (described in Section 5.5).

The Error file, called SHARC.ERR should be empty if the calculation was performed without errors or warnings. The user should always check this file to insure the calculation was performed correctly. The general output file, includes a summary of the calculation. The transmittance file contains the transmission as a function of frequency. The spectral radiance file contains the spectral radiance ($W/sr/cm^2/cm^{-1}$) as a function of frequency (cm^{-1}) and is used as an input file for the SHARC plotting package or a user provided plotting package. The SHARC plotting package is an interactive menu-query plotting package and is described in Section 6. The population file contains all of the necessary excited-state population information to allow the user to skip the population modules of SHARC and go directly to the geometry and spectral radiance modules. Populations only depend on the model atmosphere, day/night conditions, auroral parameters and solar zenith angle. Therefore, the same populations can be used for many different LOS's and bandpass configurations. This can save considerable computer time and gives the user the opportunity to develop a library of populations for future or often-used scenarios.

4.2 Sample Interactive Session

This section will feature an illustrative interactive session with the SHARC input module. The prompts from SHARC are capitalized. User responses are contained in braces, { }. Text which is inserted in to the session to clarify user responses will be contained in < >.

In the interactive execution mode SHARC looks for the "SHARC.INP" input file. This file contains the user-supplied input parameters for SHARC (several of these files are supplied on the SHARC computer tape and discussed in the test case section of this manual). If "SHARC.INP" is not found, the input module will use a set of default values for all input parameters. Once SHARC has a set of input parameters, the input module displays the top-level input menu and the user can begin to set-up a new SHARC calculation. In this example, the initial default version of 'SHARC.INP' is listed in Table 11. After the user exits the interactive input module an new version of "SHARC.INP" is saved, this file is reproduced in Table 12.

Begin session:

{run SHARC}

<The main routine successfully opens the input file >
<called SHARC.INP and the main menu is displayed. >

STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

REVIEW OR MODIFY INPUT PARAMETERS

1) TITLE FOR CALCULATION
2) REGION DEFINITION
3) LOS GEOMETRY
4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
5) SOLAR ZENITH ANGLE
6) OUTPUT DATA
7) STANDARD SET-UP FOR FILE NAMES

8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
9) EXIT WITH NO UPDATE OF DEFAULT FILE

```
ENTER # OF ITEM TO BE CHANGED OR
0 TO CONTINUE SHARC EXECUTION

       <The user can enter a number from 1 to 7 to enter a          >
       <submenu on topics 1 through 7.  Or by entering a value      >
       <of 8 the user can exit the input menu and update the        >
       <"SHARC.INP" file for a batch calculation.  Entering         >
       <a 9 will exit the sharc calculation without changing        >
       <the "SHARC.INP" file (used to quit SHARC when many input    >
       <parameters have been incorrectly entered) and entering a    >
       <0 will allow SHARC to continue interactive execution.       >
       <In this session we will start by entering a new title for   >
       <the calculation.                                            >

       <When entering a submenu the current values of parameters    >
       <are displayed.  Then the user is given the                  >
       <opportunity to keep the current values and return to the    >
       <main menu, or change the parameter values.                  >

       <The user types a 1 and enters the title submenu.            >

{1}

      1) REVIEW OR MODIFY TITLE:

          TITLE =   OLD title

    ENTER  0 TO KEEP CURRENT TITLE OR
           1 TO INPUT NEW TITLE

{1}
      INPUT TITLE:
{NEW Title}
       <The users enters a new title.                               >

      1) REVIEW OR MODIFY TITLE:

          TITLE = NEW Title

      ENTER  0 TO KEEP CURRENT TITLE OR
             1 TO INPUT NEW TITLE

       <The user moves back up to the top menu by typing a 0.       >

{0}
```

```
      STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

      REVIEW OR MODIFY INPUT PARAMETERS

    1) TITLE FOR CALCULATION
    2) REGION DEFINITION
    3) LOS GEOMETRY
    4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
    5) SOLAR ZENITH ANGLE
    6) OUTPUT DATA
    7) STANDARD SET-UP FOR FILE NAMES

    8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
    9) EXIT WITH NO UPDATE OF DEFAULT FILE

    ENTER # OF ITEM TO BE CHANGED OR
    0 TO CONTINUE SHARC EXECUTION

           <Entering a 2 the user enters the most complicated submenu  >
           <in SHARC-2, the region definition submenu.                 >
{2}

     2) REVIEW OR MODIFY REGION DEFINITIONS

        CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

       1. EXTENDED REGION IS AMBIENT
          AMBIENT MOLECULAR RADIATORS ARE CO2 NO
          MODEL ATMOSPHERE IS NIG76.DAT

       ENTER # OF REGION TO REVIEW OR MODIFY OR
            -# TO DELETE REGION OR
             2 TO ADD REGION OR
             0 TO CONTINUE
{1}
           <By entering a 1 the user can examine and/or change the     >
           <parameters which define region 1.                          >

            REGION DEFINITION DATA FOR REGION # 1

         1- REGION IS AMBIENT
         2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
         3- MONTE CARLO RADIATION TRANSPORT INPUTS
             NUMBER OF TRIAL PHOTONS       20000
             MAXIMUM ORDER OF SCATTERING     200
             SUNSHINE                         NO
             EARTHSHINE                      YES
         4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
             AMBIENT: CO2 NO
```

```
     5- NEW AMBIENT POPULATION FILE IS NIGHT.POP
   ENTER # OF ITEM TO CHANGE OR
         0 TO CONTINUE
{0}

  2) REVIEW OR MODIFY REGION DEFINITIONS

    CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

   1. EXTENDED REGION IS AMBIENT
      AMBIENT MOLECULAR RADIATORS ARE CO2 NO
      MODEL ATMOSPHERE IS NIG76.DAT

   ENTER # OF REGION TO REVIEW OR MODIFY OR
        -# TO DELETE REGION OR
         2 TO ADD REGION OR
         0 TO CONTINUE
{2}
       <By entering a 2 the user is prompted for the necessary     >
       <data to define a new region.                               >

      NEW REGION PARAMETERS FOR REGION #  2
     1- REGION ENVIRONMENT
     2- MODEL ATMOSPHERE FILE NAME
     3- MONTE CARLO RADIATION TRANSPORT INPUTS
     4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
     5- AURORAL MODEL PARAMETERS
     6- NEW POPULATION FILE NAME(S)
     7- REGION BOUNDARIES

  ENTER # OF ITEM TO INPUT DATA OR
        0 TO CONTINUE
{1}

  ENTER 1 FOR AURORAL ENVIRONMENT OR
        0 FOR AMBIENT ENVIRONMENT
{1}
       <The user selects an auroral environment.                   >

      NEW REGION PARAMETERS FOR REGION #  2
     1- REGION IS AURORAL
     2- MODEL ATMOSPHERE FILE NAME
     3- MONTE CARLO RADIATION TRANSPORT INPUTS
     4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
     5- AURORAL MODEL PARAMETERS
     6- NEW POPULATION FILE NAME(S)
     7- REGION BOUNDARIES

  ENTER # OF ITEM TO INPUT DATA OR
```

```
          O TO CONTINUE
{2}

     ENTER NEW MODEL ATMOSPHERE FILE NAME OR
     O TO RETAIN CURRENT FILE NAME
{NIG76.DAT}

           MODEL ATMOSPHERE FILE NAME IS NIG76.DAT

     ENTER NEW MODEL ATMOSPHERE FILE NAME OR
     O TO RETAIN CURRENT FILE NAME
{0}

         NEW REGION PARAMETERS FOR REGION #  2
        1- REGION IS AURORAL
        2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
        3- MONTE CARLO RADIATION TRANSPORT INPUTS
        4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
        5- AURORAL MODEL PARAMETERS
        6- NEW POPULATION FILE NAME(S)
        7- REGION BOUNDARIES

    ENTER # OF ITEM TO INPUT DATA OR
          O TO CONTINUE
{3}
         1-- NUMBER OF TRIAL PHOTONS      20000
         2-- MAXIMUM ORDER OF SCATTERING    200
         3-- SUNSHINE                       NO
         4-- EARTHSHINE                     YES
          <The above Monte Carlo input parameters are the default      >
          <values for a new region.  The user in this case wishes      >
          <to exclude excitation due to earthshine.                    >

     ENTER # OF ITEM TO BE CHANGED
     O TO CONTINUE
{4}

     DO YOU WANT EARTHSHINE ?
     ENTER 1 FOR YES OR
           O FOR NO
{0}
         1-- NUMBER OF TRIAL PHOTONS      20000
         2-- MAXIMUM ORDER OF SCATTERING    200
         3-- SUNSHINE                       NO
         4-- EARTHSHINE                     NO

     ENTER # OF ITEM TO BE CHANGED
     O TO CONTINUE
{0}
```

```
      NEW REGION PARAMETERS FOR REGION #  2
     1- REGION IS AURORAL
     2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
     3- MONTE CARLO RADIATION TRANSPORT INPUTS
        NUMBER OF TRIAL PHOTONS       20000
        MAXIMUM ORDER OF SCATTERING    200
        SUNSHINE                       NO
        EARTHSHINE                     NO
     4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
     5- AURORAL MODEL PARAMETERS
     6- NEW POPULATION FILE NAME(S)
     7- REGION BOUNDARIES

 ENTER # OF ITEM TO INPUT DATA OR
       0 TO CONTINUE
{4}
       <The user is going to add NO as a species to both the        >
       <ambient and auroral environments.                           >

  ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
      - MOLECULAR FORMULA TO REMOVE SPECIES
      0 TO CONTINUE
{NO}

     ADDING INPUT DATA FOR NO

 1   ADD SPECIES TO AMBIENT ENVIRONMENT
 2   ADD SPECIES TO AURORAL ENVIRONMENT

  ENTER # OF ITEM TO CHANGE OR
        0 TO CONTINUE
{1}

 ENTER AMBIENT LINKING FILE NAME
{NOLINK.DAT}

 ENTER AMBIENT  STATES FILE NAME
{NOSTAT.DAT}

 ENTER AMBIENT   BANDS FILE NAME
{NOBAND.DAT}

     REVIEW OF NO    INPUT DATA
     AMBIENT DATA
 #   ISOTOPE             LINKING              STATES               BANDS
 1   14N 16O              NOLINK.DAT          NOSTAT.DAT           NOBAND.DAT

 2   ADD SPECIES TO AURORAL ENVIRONMENT
```

```
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{2}

     ENTER AURORAL LINKING FILE NAME
{ANOLINK.DAT}

     ENTER AURORAL  STATES FILE NAME
{ANOSTAT.DAT}

         REVIEW OF NO    INPUT DATA
         AMBIENT DATA
     #   ISOTOPE              LINKING              STATES                BANDS
     1   14N 16O               NOLINK.DAT          NOSTAT.DAT           NOBAND.DAT
         AURORAL DATA
     #   ISOTOPE              LINKING              STATES
     2   14N 16O              ANOLINK.DAT         ANOSTAT.DAT

           <Notice that auroral species do not require a BANDS file.  >
           <At this point the user has successfully added NO to       >
           <both environments.                                        >

      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{0}

          AMBIENT RADIATORS ARE:
                   NO    ISOTOPE   14N 16O

          AURORAL RADIATORS ARE:
                   NO    ISOTOPE   14N 16O

      ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
          - MOLECULAR FORMULA TO REMOVE SPECIES
          0 TO CONTINUE

           <Adding NO+ to on.  the auroral environment.               >
{no+}

         ADDING INPUT DATA FOR NO+

     1   ADD SPECIES TO AMBIENT ENVIRONMENT
     2   ADD SPECIES TO AURORAL ENVIRONMENT

      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{2}
```

```
     ENTER AURORAL LINKING FILE NAME
{ANO+LINK.DAT}

     ENTER AURORAL  STATES FILE NAME
{ANO+STAT.DAT}

         REVIEW OF NO+   INPUT DATA
         AURORAL DATA
     #   ISOTOPE              LINKING               STATES
     1   14N 16O            ANO+LINK.DAT          ANO+STAT.DAT

     2   ADD SPECIES TO AMBIENT ENVIRONMENT

      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{0}

          AMBIENT RADIATORS ARE:
                   NO    ISOTOPE   14N 16O

          AURORAL RADIATORS ARE:
                   NO    ISOTOPE   14N 16O
                   NO+   ISOTOPE   14N 16O

      ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
        - MOLECULAR FORMULA TO REMOVE SPECIES
        0 TO CONTINUE
{co2}

         ADDING INPUT DATA FOR CO2

     1   ADD SPECIES TO AMBIENT ENVIRONMENT
     2   ADD SPECIES TO AURORAL ENVIRONMENT

      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{1}

       ISOTOPES INCLUDE:
         AFGL ISO# 1 NAME 16O 12C 16O
         AFGL ISO# 2 NAME 16O 13C 16O
         AFGL ISO# 3 NAME 16O 12C 18O
         AFGL ISO# 4 NAME 16O 12C 17O
         AFGL ISO# 5 NAME 16O 13C 18O
         AFGL ISO# 6 NAME 16O 13C 17O
         AFGL ISO# 7 NAME 18O 12C 18O
         AFGL ISO# 8 NAME 17O 12C 18O

      ENTER ISOTOPE NUMBER OR
```

```
     0 TO CONTINUE

          <CO2 has several isotopes which are supported by SHARC-2.   >
          <The user must select the isotope desired from the list of  >
          <supported isotopes.  In this case the user selects a 1 for >
          <the most abundant isotope, 16O12C16O.                      >
{1}
          <The isotopes each have their own linking, states and bands >
          <files.  They are labeled with the AFGL isotope number in   >
          <the filenames.  For example, CO21LINK.DAT is the linking   >
          <file for the most abundant isotope of CO2.                 >

     ENTER AMBIENT LINKING FILE NAME
{CO21LINK.DAT}

     ENTER AMBIENT  STATES FILE NAME
{CO21STAT.DAT}

     ENTER AMBIENT   BANDS FILE NAME
{CO21BAND.DAT}

       ISOTOPES INCLUDE:
         AFGL ISO# 2 NAME 16O 13C 16O
         AFGL ISO# 3 NAME 16O 12C 18O
         AFGL ISO# 4 NAME 16O 12C 17O
         AFGL ISO# 5 NAME 16O 13C 18O
         AFGL ISO# 6 NAME 16O 13C 17O
         AFGL ISO# 7 NAME 18O 12C 18O
         AFGL ISO# 8 NAME 17O 12C 18O

      ENTER ISOTOPE NUMBER OR
      0 TO CONTINUE
{0}

         REVIEW OF CO2   INPUT DATA
         AMBIENT DATA
     #   ISOTOPE             LINKING             STATES              BANDS
     1 16O 12C 16O         CO21LINK.DAT        CO21STAT.DAT        CO21BAND.DAT

     2   ADD SPECIES TO AMBIENT ENVIRONMENT
     3   ADD SPECIES TO AURORAL ENVIRONMENT

      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{0}


          AMBIENT RADIATORS ARE:
                   NO   ISOTOPE   14N 16O
```

```
              CO2  ISOTOPE 16O 12C 16O

          AURORAL RADIATORS ARE:
                   NO   ISOTOPE   14N 16O
                   NO+  ISOTOPE   14N 16O

      ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
          - MOLECULAR FORMULA TO REMOVE SPECIES
          0 TO CONTINUE
{0}

          NEW REGION PARAMETERS FOR REGION #  2
         1- REGION IS AURORAL
         2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
         3- MONTE CARLO RADIATION TRANSPORT INPUTS
             NUMBER OF TRIAL PHOTONS      20000
             MAXIMUM ORDER OF SCATTERING   200
             SUNSHINE                      NO
             EARTHSHINE                    NO
         4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
             AMBIENT: NO  CO2
             AURORAL: NO  NO+ CO2
         5- AURORAL MODEL PARAMETERS
         6- NEW POPULATION FILE NAME(S)
         7- REGION BOUNDARIES

     ENTER # OF ITEM TO INPUT DATA OR
           0 TO CONTINUE
           <The user now defines the auroral conditions desired for    >
           <the simulation.                                            >
{5}

         AURORAL MODEL PARAMETERS

         1--INCIDENT ELECTRON ENERGY SPECTRUM
         2--DURATION OF AURORA IS     0.0 SEC
         3--TIME OF OBSERVATION IS     0.0 SEC

       ENTER # OF ITEM TO CHANGE OR
             0 TO CONTINUE
{1}

          CHOOSE EITHER :

        1 - CODE DEFINED INCIDENT ELECTRON ENERGY SPECTRUM
        2 - USER DEFINED INCIDENT ELECTRON ENERGY SPECTRUM

       ENTER # OF ITEM TO BE CHANGED
{1}
```

```
        CODE SUPPLIED INCIDENT ELECTRON ENERGY SPECTRA

         IBC INDEX    /    MAXWELLIAN DISTRIBUTION    /
                      /                               /
                      / FLUX(ERGS/CM2/S)  ENERGY(KEV) /
         2 - IBC II   /        12.9           2.9     /
         3 - IBC III  /       100.0           5.0     /
         4 - IBC III+ /       400.0          10.0     /


       SELECT AURORAL INDEX
{3}

          AURORAL MODEL PARAMETERS

          1--INCIDENT ELECTRON ENERGY SPECTRUM
              IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
              TOTAL ENERGY FLUX IS   100.0 ERGS/CM2/S
              CHARACTERISTIC ENERGY IS     5.0 KEV
          2--DURATION OF AURORA IS     0.0 SEC
          3--TIME OF OBSERVATION IS     0.0 SEC

        ENTER # OF ITEM TO CHANGE OR
              0 TO CONTINUE
{2}

       INPUT AURORA DURATION IN SECONDS:
{100}

          AURORAL MODEL PARAMETERS

          1--INCIDENT ELECTRON ENERGY SPECTRUM
              IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
              TOTAL ENERGY FLUX IS   100.0 ERGS/CM2/S
              CHARACTERISTIC ENERGY IS     5.0 KEV
          2--DURATION OF AURORA IS   100.0 SEC
          3--TIME OF OBSERVATION IS     0.0 SEC

        ENTER # OF ITEM TO CHANGE OR
              0 TO CONTINUE
{3}

       INPUT RELATIVE TIME OF OBSERVATION IN SECONDS:
{100}

          AURORAL MODEL PARAMETERS

          1--INCIDENT ELECTRON ENERGY SPECTRUM
```

```
          IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
          TOTAL ENERGY FLUX IS    100.0 ERGS/CM2/S
          CHARACTERISTIC ENERGY IS      5.0 KEV
      2--DURATION OF AURORA IS    100.0 SEC
      3--TIME OF OBSERVATION IS    100.0 SEC

    ENTER # OF ITEM TO CHANGE OR
          0 TO CONTINUE
{0}

       NEW REGION PARAMETERS FOR REGION #  2
      1- REGION IS AURORAL
      2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
      3- MONTE CARLO RADIATION TRANSPORT INPUTS
          NUMBER OF TRIAL PHOTONS       20000
          MAXIMUM ORDER OF SCATTERING    200
          SUNSHINE                       NO
          EARTHSHINE                     NO
      4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
          AMBIENT: NO  CO2
          AURORAL: NO  NO+ CO2
      5- REVIEW OR MODIFY AURORAL MODEL PARAMETERS
          IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
          TOTAL ENERGY FLUX IS    100.0 ERGS/CM2/S
          CHARACTERISTIC ENERGY IS      5.0 KEV
          DURATION OF AURORA IS    100.0 SEC WITH OBSERVATION AT    100.0 SEC
      6- NEW POPULATION FILE NAME(S)
      7- REGION BOUNDARIES

  ENTER # OF ITEM TO INPUT DATA OR
        0 TO CONTINUE
{6}

         POPULATION FILE NAME(S) AND STATUS
       1-AMBIENT POPULATION FILE NAME
       2-FILE IS NEW AND NOT CURRENTLY SAVED
       3-AURORAL POPULATION FILE NAME
       4-FILE IS NEW AND NOT CURRENTLY SAVED
   ENTER # OF ITEM TO CHANGE OR
         0 TO CONTINUE

        <When performing an auroral calculation the user defines    >
        <two population files.  One population file does/or will    >
        <contain the ambient population which will be enhanced by   >
        <the aurora.  The second population file contains the       >
        <aurorally enhanced populations and other necessary auroral >
        <information.  The ambient population file can either be    >
        <new or old, previously calculated, in this example we will >
        <be using the population file generated in the region one   >
```

```
          <calculation.  The auroral population file can also be      >
          <either new or old, with a new file being calculated in this>
          <example.  The population files for different environments  >
          <contains different information, therefore an auroral       >
          <population file must be used in an auroral calculation.    >
          <Considerable computational time can be saved by using old  >
          <population files since over half of the time in a single   >
          <region SHARC-2 calculation is used in generating the       >
          <populations.                                               >

{1}

      ENTER AMBIENT POPULATION FILE NAME
{NIGHT.POP}

            POPULATION FILE NAME(S) AND STATUS
          1-AMBIENT POPULATION FILE NAME IS NIGHT.POP
          2-FILE IS NEW AND NOT CURRENTLY SAVED
          3-AURORAL POPULATION FILE NAME IS UNKNOWN
          4-FILE IS NEW AND NOT CURRENTLY SAVED
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{2}

      ENTER 0 TO NOT SAVE POPULATION FILE
            1 TO SAVE NEW POPULATION FILE
            2 TO USE OLD POPULATION FILE
{2}

            POPULATION FILE NAME(S) AND STATUS
          1-AMBIENT POPULATION FILE NAME IS NIGHT.POP
          2-FILE STATUS IS OLD
          3-AURORAL POPULATION FILE NAME IS UNKNOWN
          4-FILE IS NEW AND NOT CURRENTLY SAVED
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{3}

      ENTER AURORAL POPULATION FILE NAME
{ANIGHT.POP}

            POPULATION FILE NAME(S) AND STATUS
          1-AMBIENT POPULATION FILE NAME IS NIGHT.POP
          2-FILE STATUS IS OLD
          3-AURORAL POPULATION FILE NAME IS ANIGHT.POP
          4-FILE IS NEW AND NOT CURRENTLY SAVED
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{4}
```

```
      ENTER 0 TO NOT SAVE POPULATION FILE
            1 TO SAVE NEW POPULATION FILE
            2 TO USE OLD POPULATION FILE
{1}

            POPULATION FILE NAME(S) AND STATUS
          1-AMBIENT POPULATION FILE NAME IS NIGHT.POP
          2-FILE STATUS IS OLD
          3-AURORAL POPULATION FILE NAME IS ANIGHT.POP
          4-FILE STATUS IS NEW
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{0}

          NEW REGION PARAMETERS FOR REGION #  2
         1- REGION IS AURORAL
         2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
         3- MONTE CARLO RADIATION TRANSPORT INPUTS
             NUMBER OF TRIAL PHOTONS      20000
             MAXIMUM ORDER OF SCATTERING   200
             SUNSHINE                      NO
             EARTHSHINE                    NO
         4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
             AMBIENT: NO  CO2
             AURORAL: NO  NO+ CO2
         5- REVIEW OR MODIFY AURORAL MODEL PARAMETERS
             IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
             TOTAL ENERGY FLUX IS   100.0 ERGS/CM2/S
             CHARACTERISTIC ENERGY IS      5.0 KEV
             DURATION OF AURORA IS   100.0 SEC WITH OBSERVATION AT   100.0 SEC
         6- OLD AMBIENT POPULATION FILE IS NIGHT.POP
            NEW AURORAL POPULATION FILE IS ANIGHT.POP
         7- REGION BOUNDARIES

     ENTER # OF ITEM TO INPUT DATA OR
           0 TO CONTINUE
           <Define local region.                                              >
{7}
           REGION BOUNDARIES
         1-LOCATION OF ORIGIN
         2-UPPER ALTITUDE FOR REGION
         3-LOWER ALTITUDE FOR REGION
         4-CORNERS OF REGION
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
{1}

      ORIGIN OF REGION COORDINATE SYSTEM
      ENTER 1 FOR MAGNETIC NORTH POLE OR
```

```
          0 FOR GEOGRAPHIC NORTH POLE
{0}

          REGION BOUNDARIES
       1-ORIGIN AT GEOGRAPHIC NORTH POLE
       2-UPPER ALTITUDE FOR REGION IS      0.00 KM
       3-LOWER ALTITUDE FOR REGION IS      0.00 KM
       4-CORNERS OF REGION
           CORNER #      LATITUDE       LONGITUDE
               1           0.00           0.00
               2           0.00           0.00
               3           0.00           0.00
               4           0.00           0.00
    ENTER # OF ITEM TO CHANGE OR
          0 TO CONTINUE
{2}

    ENTER UPPER ALTITUDE OF REGION IN KM
{120}

          REGION BOUNDARIES
       1-ORIGIN AT GEOGRAPHIC NORTH POLE
       2-UPPER ALTITUDE FOR REGION IS    120.00 KM
       3-LOWER ALTITUDE FOR REGION IS      0.00 KM
       4-CORNERS OF REGION
           CORNER #      LATITUDE       LONGITUDE
               1           0.00           0.00
               2           0.00           0.00
               3           0.00           0.00
               4           0.00           0.00
    ENTER # OF ITEM TO CHANGE OR
          0 TO CONTINUE
{3}

    ENTER LOWER ALTITUDE OF REGION IN KM
{80}

          REGION BOUNDARIES
       1-ORIGIN AT GEOGRAPHIC NORTH POLE
       2-UPPER ALTITUDE FOR REGION IS    120.00 KM
       3-LOWER ALTITUDE FOR REGION IS     80.00 KM
       4-CORNERS OF REGION
           CORNER #      LATITUDE       LONGITUDE
               1           0.00           0.00
               2           0.00           0.00
               3           0.00           0.00
               4           0.00           0.00
    ENTER # OF ITEM TO CHANGE OR
          0 TO CONTINUE
```

```
{4}

      ENTER FOUR LATITUDE AND LONGITUDE PAIRS
     ENTER LATITUDE FOR CORNER # 1 IN DEGREES
{5}
     ENTER LONGITUDE FOR CORNER # 1 IN DEGREES
{5}
     ENTER LATITUDE FOR CORNER # 2 IN DEGREES
{5}
     ENTER LONGITUDE FOR CORNER # 2 IN DEGREES
{355}
     ENTER LATITUDE FOR CORNER # 3 IN DEGREES
{-5}
     ENTER LONGITUDE FOR CORNER # 3 IN DEGREES
{355}
 ENTER LATITUDE FOR CORNER # 4 IN DEGREES
{-5}
     ENTER LONGITUDE FOR CORNER # 4 IN DEGREES
{5}

            REGION BOUNDARIES
         1-ORIGIN AT GEOGRAPHIC NORTH POLE
         2-UPPER ALTITUDE FOR REGION IS   120.00 KM
         3-LOWER ALTITUDE FOR REGION IS    80.00 KM
         4-CORNERS OF REGION
             CORNER #      LATITUDE      LONGITUDE
                 1            5.00           5.00
                 2            5.00         355.00
                 3           -5.00         355.00
                 4           -5.00           5.00
      ENTER # OF ITEM TO CHANGE OR
            0 TO CONTINUE
           <The user has defined a local region which extends from    >
           <80 to 120 km altitude and is centered over the equator    >
           <between 5 and 355 longitude.                              >
{0}

          NEW REGION PARAMETERS FOR REGION #  2
         1- REGION IS AURORAL
         2- MODEL ATMOSPHERE FILE NAME IS NIG76.DAT
         3- MONTE CARLO RADIATION TRANSPORT INPUTS
             NUMBER OF TRIAL PHOTONS       20000
             MAXIMUM ORDER OF SCATTERING    200
             SUNSHINE                        NO
             EARTHSHINE                      NO
         4- MOLECULAR RADIATORS FOR POPULATION CALCULATION
             AMBIENT: NO  CO2
             AURORAL: NO  NO+
```

```
        5- REVIEW OR MODIFY AURORAL MODEL PARAMETERS
            IBC TYPE III AURORA (MAXWELLIAN DISTRIBUTION)
            TOTAL ENERGY FLUX IS    100.0 ERGS/CM2/S
            CHARACTERISTIC ENERGY IS      5.0 KEV
            DURATION OF AURORA IS    100.0 SEC WITH OBSERVATION AT    100.0 SEC
        6- OLD AMBIENT POPULATION FILE IS NIGHT.POP
           NEW AURORAL POPULATION FILE IS ANIGHT.POP
        7- REGION BOUNDARIES

    ENTER # OF ITEM TO INPUT DATA OR
          0 TO CONTINUE
{0}

    2) REVIEW OR MODIFY REGION DEFINITIONS

        CURRENTLY THERE ARE  2 REGIONS: 1 EXTENDED AND  1 LOCAL

      1. EXTENDED REGION IS AMBIENT
         AMBIENT MOLECULAR RADIATORS ARE CO2 NO
         MODEL ATMOSPHERE IS NIG76.DAT
      2. LOCAL REGION IS AURORAL
         USING OLD AMBIENT POPULATION FILE CALLED NIGHT.POP
         AURORAL MOLECULAR RADIATORS ARE NO  NO+
         MODEL ATMOSPHERE IS NIG76.DAT

      ENTER # OF REGION TO REVIEW OR MODIFY OR
           -# TO DELETE REGION OR
            3 TO ADD REGION OR
            0 TO CONTINUE
{0}
          <Exit region menu to continue session at top menu.          >

     STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

     REVIEW OR MODIFY INPUT PARAMETERS

     1) TITLE FOR CALCULATION
     2) REGION DEFINITION
     3) LOS GEOMETRY
     4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
     5) SOLAR ZENITH ANGLE
     6) OUTPUT DATA
     7) STANDARD SET-UP FOR FILE NAMES

     8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
     9) EXIT WITH NO UPDATE OF DEFAULT FILE

     ENTER # OF ITEM TO BE CHANGED OR
     0 TO CONTINUE SHARC EXECUTION
```

```
{2}
     3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

       CURRENT VALUES ARE:
       1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NORTH POLE
       2. ASSUMING SPHERICAL EARTH
       3. PATH TYPE IS LIMB VIEWING PATH
           OBSERVER INFORMATION
           TANGENT HEIGHT:        100.0000     KM
           TANGENT LONGITUDE:       0.0000000E+00 DEGREES
           TANGENT LATITUDE:        0.0000000E+00 DEGREES

            LOCAL AZIMUTH AT TANGENT POINT
            AZIMUTH ANGLE:      0.0000000E+00 DEGREES

     ENTER # OF ITEM TO CHANGE OR
           0 TO CONTINUE
{3}
        PATH TYPES
        2 -- OBSERVER TO SOURCE POINT
        3 -- OBSERVER TO SPACE
        4 -- LIMB VIEWING PATH
     SELECT PATH TYPE (0 TO KEEP CURRENT INFORMATION)
{4}
     INPUT TANGENT HEIGHT IN KM
{80}
     INPUT TANGENT POINT LONGITUDE IN DEGREES
{0}
     INPUT TANGENT POINT LATITUDE IN DEGREES
{0}

     LOCAL AZIMUTH AT TANGENT POINT
     ENTER 0 FOR DIRECT INPUT OF AZIMUTH ANGLE
           1 TO FORCE LOS THRU A POINT TOWARD TANGENT POINT
           2 TO FORCE LOS THRU A POINT BEHIND TANGENT POINT
{0}

     INPUT AZIMUTH ANGLE IN DEGREES
{0}

     3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

       CURRENT VALUES ARE:
       1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NORTH POLE
       2. ASSUMING SPHERICAL EARTH
       3. PATH TYPE IS LIMB VIEWING PATH
           OBSERVER INFORMATION
           TANGENT HEIGHT:        80.00000     KM
```

TANGENT LONGITUDE: 0.0000000E+00 DEGREES
TANGENT LATITUDE: 0.0000000E+00 DEGREES

LOCAL AZIMUTH AT TANGENT POINT
AZIMUTH ANGLE: 0.0000000E+00 DEGREES

ENTER # OF ITEM TO CHANGE OR
0 TO CONTINUE

{0}

<The user has selected a new limb viewing line-of-sight >
<with a tangent height of 80 km and passing through >
<0 longitude and 0 latitude. To fully specify the LOS >
<the user must still specify either a point along the LOS >
<trajectory, or the azimuth angle at the tangent point. >

STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

REVIEW OR MODIFY INPUT PARAMETERS

1) TITLE FOR CALCULATION
2) REGION DEFINITION
3) LOS GEOMETRY
4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
5) SOLAR ZENITH ANGLE
6) OUTPUT DATA
7) STANDARD SET-UP FOR FILE NAMES

8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
9) EXIT WITH NO UPDATE OF DEFAULT FILE

ENTER # OF ITEM TO BE CHANGED OR
0 TO CONTINUE SHARC EXECUTION

{4}

<The user wants to calculate the spectral emission from NO, >
<NO+ and CO_2 from 250 to 5000 cm^{-1} at 2 cm^{-1} resolution. >

4) REVIEW OR MODIFY SPECTRAL INPUTS...

CURRENT VALUES ARE:
1. MINIMUM WAVENUMBER : 3000.000
2. MAXIMUM WAVENUMBER : 4000.000
3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) : 1.000000
4. SPECIES INCLUDED IN RADIANCE CALCULATION

CO2	ISOTOPE	16O 12C 16O	AFGL ISOTOPE #	1
NO	ISOTOPE	14N 16O	AFGL ISOTOPE #	1

ENTER # OF ITEM TO BE CHANGED OR
0 TO CONTINUE

{1}

```
        INPUT MINIMUM OF SPECTRAL INTERVAL IN WAVENUMBERS
{250}
            CURRENT VALUES ARE:
         1. MINIMUM WAVENUMBER :      250.0000
         2. MAXIMUM WAVENUMBER :      4000.000
         3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) :      1.000000
         4. SPECIES INCLUDED IN RADIANCE CALCULATION
                    CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1
                    NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1

        ENTER # OF ITEM TO BE CHANGED OR
              0 TO CONTINUE
{2}
         INPUT MAXIMUM OF SPECTRAL INTERVAL IN WAVENUMBERS
{5000}
            CURRENT VALUES ARE:
         1. MINIMUM WAVENUMBER :      250.0000
         2. MAXIMUM WAVENUMBER :      5000.000
         3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) :      1.000000
         4. SPECIES INCLUDED IN RADIANCE CALCULATION
                    CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1
                    NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1

        ENTER # OF ITEM TO BE CHANGED OR
              0 TO CONTINUE
{3}
         INPUT SPECTRAL RESOLUTION IN WAVENUMBERS
{2}
            CURRENT VALUES ARE:
         1. MINIMUM WAVENUMBER :      250.0000
         2. MAXIMUM WAVENUMBER :      5000.000
         3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) :      2.000000
         4. SPECIES INCLUDED IN RADIANCE CALCULATION
                    CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1
                    NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1

        ENTER # OF ITEM TO BE CHANGED OR
              0 TO CONTINUE
{4}

           CURRENT SPECIES ARE :
                    CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1
                    NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1

       ENTER NEW SPECIES MOLECULAR FORMULA OR
           - MOLECULAR FORMULA TO REMOVE SPECIES
           0 TO CONTINUE
{[illegible]}
```

```
          CURRENT SPECIES ARE :
                   CO2   ISOTOPE 16O 12C 16O    AFGL ISOTOPE #  1
                   NO    ISOTOPE   14N 16O      AFGL ISOTOPE #  1
                   NO+   ISOTOPE   14N 16O      AFGL ISOTOPE #  1

      ENTER NEW SPECIES MOLECULAR FORMULA OR
          - MOLECULAR FORMULA TO REMOVE SPECIES
          0 TO CONTINUE
{0}
           CURRENT VALUES ARE:
        1. MINIMUM WAVENUMBER :      250.0000
        2. MAXIMUM WAVENUMBER :      5000.000
        3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) :      2.000000
        4. SPECIES INCLUDED IN RADIANCE CALCULATION
                   CO2   ISOTOPE 16O 12C 16O    AFGL ISOTOPE #  1
                   NO    ISOTOPE   14N 16O      AFGL ISOTOPE #  1
                   NO+   ISOTOPE   14N 16O      AFGL ISOTOPE #  1

       ENTER # OF ITEM TO BE CHANGED OR
             0 TO CONTINUE
{4}

          CURRENT SPECIES ARE :
                   CO2   ISOTOPE 16O 12C 16O    AFGL ISOTOPE #  1
                   NO    ISOTOPE   14N 16O      AFGL ISOTOPE #  1
                   NO+   ISOTOPE   14N 16O      AFGL ISOTOPE #  1

      ENTER NEW SPECIES MOLECULAR FORMULA OR
          - MOLECULAR FORMULA TO REMOVE SPECIES
          0 TO CONTINUE
{-co2}
           <We have deleted CO2, just to demonstrate the                 >
           <removal process.                                             >

          CURRENT SPECIES ARE :
                   NO    ISOTOPE   14N 16O      AFGL ISOTOPE #  1
                   NO+   ISOTOPE   14N 16O      AFGL ISOTOPE #  1

      ENTER NEW SPECIES MOLECULAR FORMULA OR
          - MOLECULAR FORMULA TO REMOVE SPECIES
          0 TO CONTINUE
           <When adding CO2 back into the species list there are 8       >
           <isotopes supported by SHARC-2.  In this example we want      >
           <emission from only the major isotope #1.                     >

{CO2}
       ISOTOPES INCLUDE:
         AFGL ISO# 1 NAME 16O 12C 16O
         AFGL ISO# 2 NAME 16O 13C 16O
```

```
     AFGL ISO# 3 NAME 16O 12C 18O
     AFGL ISO# 4 NAME 16O 12C 17O
     AFGL ISO# 5 NAME 16O 13C 18O
     AFGL ISO# 6 NAME 16O 13C 17O
     AFGL ISO# 7 NAME 18O 12C 18O
     AFGL ISO# 8 NAME 17O 12C 18O

  ENTER ISOTOPE NUMBER OR
  0 TO CONTINUE
{1}

   ISOTOPES INCLUDE:
     AFGL ISO# 2 NAME 16O 13C 16O
     AFGL ISO# 3 NAME 16O 12C 18O
     AFGL ISO# 4 NAME 16O 12C 17O
     AFGL ISO# 5 NAME 16O 13C 18O
     AFGL ISO# 6 NAME 16O 13C 17O
     AFGL ISO# 7 NAME 18O 12C 18O
     AFGL ISO# 8 NAME 17O 12C 18O

  ENTER ISOTOPE NUMBER OR
  0 TO CONTINUE
{0}

      CURRENT SPECIES ARE :
             NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1
             NO+  ISOTOPE   14N 16O     AFGL ISOTOPE #  1
             CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1

  ENTER NEW SPECIES MOLECULAR FORMULA OR
      - MOLECULAR FORMULA TO REMOVE SPECIES
      0 TO CONTINUE
{0}
       CURRENT VALUES ARE:
    1. MINIMUM WAVENUMBER :      250.0000
    2. MAXIMUM WAVENUMBER :      5000.000
    3. SPECTRAL RESOLUTION (MINIMUM OF .1 CM-1) :      2.000000
    4. SPECIES INCLUDED IN RADIANCE CALCULATION
             NO   ISOTOPE   14N 16O     AFGL ISOTOPE #  1
             NO+  ISOTOPE   14N 16O     AFGL ISOTOPE #  1
             CO2  ISOTOPE 16O 12C 16O   AFGL ISOTOPE #  1

   ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
{0}

  STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

  REVIEW OR MODIFY INPUT PARAMETERS
```

```
      1) TITLE FOR CALCULATION
      2) REGION DEFINITION
      3) LOS GEOMETRY
      4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
      5) SOLAR ZENITH ANGLE
      6) OUTPUT DATA
      7) STANDARD SET-UP FOR FILE NAMES

      8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
      9) EXIT WITH NO UPDATE OF DEFAULT FILE

      ENTER # OF ITEM TO BE CHANGED OR
      0 TO CONTINUE SHARC EXECUTION
{6}

      6) REVIEW OR MODIFY OUTPUT DESIRED...

        IWRITE VALUES RANGE FROM 0 TO 2
        LOW VALUES DECREASE THE AMOUNT OF OUTPUT
        HIGH VALUES INCLUDE ALL OUTPUT FROM LOWER VALUES
        FOR EXAMPLE: IWRITE=2 WOULD INCLUDE IWRITE=1 OUTPUT

        CURRENT VALUES ARE:
     1. MODEL ATMOSPHERE OUTPUT:                          1
     2. SELECTED TRANSITIONS:                             1
     3. MOLECULAR BAND INFORMATION:                       0
     4. NOT CURRENTLY USED:                               0
     5. NEMESIS OUTPUT:                                   0
     6. AURORAL OUTPUT:                                   1
     7. FINAL EXCITED STATE POPULATIONS:                  1
     8. EXCITED STATE VIBRATIONAL TEMPERATURES:           1
     9. LINE-OF-SIGHT OUTPUT:                             1
    10. SPECTRAL RADIANCE OUTPUT:                         0

         <This set of values will generate a fairly standard output. >
         <The output will include the model atmosphere, selected     >
         <transitions for all species, some auroral output, final    >
         <excited state population and vibrational temperatures,     >
         <and LOS and column density information.                    >


      ENTER # OF ITEM TO BE CHANGED OR
            0 TO CONTINUE
{0}

      STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

      REVIEW OR MODIFY INPUT PARAMETERS
```

```
      1) TITLE FOR CALCULATION
      2) REGION DEFINITION
      3) LOS GEOMETRY
      4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
      5) SOLAR ZENITH ANGLE
      6) OUTPUT DATA
      7) STANDARD SET-UP FOR FILE NAMES

      8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
      9) EXIT WITH NO UPDATE OF DEFAULT FILE

      ENTER # OF ITEM TO BE CHANGED OR
      0 TO CONTINUE SHARC EXECUTION
{7}

      7) REVIEW OR MODIFY STANDARD I/O FILE NAMES

        1. LINE FILE NAME IS              SHARC.LIN
        2. SPECTRAL RADIANCE FILE NAME IS SHARC.SPC
        3. TRANSMISSION FILE NAME IS      SHARC.TRN
        4. STANDARD OUTPUT FILE NAME IS   SHARC.OUT

           <SHARC-2 allows the user to input arbitrary names for the   >
           <standard output files.                                     >

      ENTER  # OF ITEM TO BE CHANGED OR
             0 TO CONTINUE

{4}
      INPUT STANDARD OUTPUT FILE NAME
{SHARCNIGHT.OUT}

      7) REVIEW OR MODIFY STANDARD I/O FILE NAMES

        1. LINE FILE NAME IS              SHARC.LIN
        2. SPECTRAL RADIANCE FILE NAME IS SHARC.SPC
        3. TRANSMISSION FILE NAME IS      SHARC.TRN
        4. STANDARD OUTPUT FILE NAME IS   SHARCNIGHT.OUT

      ENTER  # OF ITEM TO BE CHANGED OR
             0 TO CONTINUE

{0}

      STRATEGIC HIGH-ALTITUDE RADIANCE CODE, SHARC-2

      REVIEW OR MODIFY INPUT PARAMETERS
```

```
1) TITLE FOR CALCULATION
2) REGION DEFINITION
3) LOS GEOMETRY
4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
5) SOLAR ZENITH ANGLE
6) OUTPUT DATA
7) STANDARD SET-UP FOR FILE NAMES

8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
9) EXIT WITH NO UPDATE OF DEFAULT FILE

ENTER # OF ITEM TO BE CHANGED OR
0 TO CONTINUE SHARC EXECUTION
```

{8}

```
NUMBER OF INTERSECTIONS WITH LOCAL REGION  2 IS  2

POINT   RANGE   ALTITUDE  LATITUDE  LONGITUDE
  1    1132.52   104.83     -5.02      0.00
  2    2265.61   104.83      5.02      0.00

SHARC READY FOR BATCH RUN
     <The LOS selected intersects the defined local region at     >
     <two locations.  It is possible to have as many as four      >
     <intersections and as few as zero.  The user is alerted      >
     <when no intersections are found in case the desired LOS     >
     <was incorrectly entered into SHARC.                         >
```

TABLE 11. SAMPLE SHARC.INP FILE.

```
C0 STANDARD INPUT FILE SHARC.INP
C0 THIS FILE HOLDS THE DEFAULT VALUES FOR SHARC
C0 THIS FILE IS UPDATED TO THE CURRENT VALUES OF THE PARAMETERS
C0 EACH TIME SHARC IS RUN.
C0 LINES WHICH HAVE A "C" IN COLUMN 1 ARE TREATED AS COMMENT
C0
C1 THE FIRST LINE CONTAINS THE INTERACTIVE/BATCH OPTION
C1 IF IT EQUALS 1, SHARC WILL RUN INTERACTIVELY, ALLOWING
C1 THE USER TO UPDATE OPTIONS.  IF IT EQUALS 0, SHARC WILL
C1 RUN IN BATCH MODE.
C1
   1
C2 TITLE FOR CALCULATION
C2
  OLD title
C3 OUTPUT CONTROL PARAMETERS:
C3 1) MODEL ATMOSPHERE OUTPUT ==>1 FOR FULL LISTING
C3 2) SELECTED TRANSITIONS ==>1 FOR TRANSITIONS SELECTED
C3 3) MOLECULAR BAND INFORMATION ==>1 FOR BAND INFORMATION
C3 4) NOT CURRENTLY USED
C3 5) NEMESIS OUTPUT ==>1 NEMESIS ONLY ==>2 FOR POST POPULATIONS
C3 6) AURORAL OUTPUT ==>1 FINAL ONLY ==>2 TIME DEVELOPMENT
C3 7) FINAL STATE POPULATIONS ==>1 YES
C3 8) FINAL VIBRATIONAL TEMPERATURES ==>1 YES
C3 9) LOS OUTPUT ==>1 FOR COLUMN DENSITIES
C3 10)SPECTRAL RADIANCE OUTPUT ==>1 FOR RADIANCE OUTPUT
C3 1   2   3   4   5   6   7   8   9   10
   1   1   0   0   0   1   1   1   1   0
C4 FILE NAME (AND PATH) FOR SHARC LINE FILE
C4
  SHARC.LIN
C5 FILE NAME (AND PATH) FOR SHARC SPECTRAL RADIANCE OUTPUT FILE
C5
  SHARC.SPC
C6 FILE NAME (AND PATH) FOR SHARC TRANSMISSION OUTPUT FILE
C6
  SHARC.TRN
C7 FILE NAME (AND PATH) FOR SHARC GENERAL OUTPUT FILE NAME
C7
  SHARC.OUT
C8 SOLAR ZENITH ANGLE IN DEGREES
C8
```

```
  0.100000E+02
C9 LINE-OF-SIGHT INFORMATION : PATH TYPE, CASE, ORIGIN LOCATION
C9 AND SPHERICAL EARTH INDEX
C9
   4     1     0     0
C10 OBSERVER INFORMATION: ALTITUDE (KM), LONGITUDE AND LATITUDE
C10
  0.300000E+03    0.000000E+00   -0.140653E+02
C11 SOURCE INFORMATION: ALTITUDE (KM), LONGITUDE AND LATITUDE
C11
  0.300000E+03    0.000000E+00    0.140653E+02
C12 TANGENT ALTITUDE, LONGITUDE AND LATITUDE AT TANGENT POINT
C12
  0.100000E+03    0.000000E+00    0.000000E+00
C13 LOS CASE INDEX, LONGITUDE AND LATITUDE ALONG LOS VECTOR
C13
     0  0.000000E+00  0.000000E+00
C14 ZENITH ANGLE, AZIMUTH ANGLE, OBSERVER-EARTH-SOURCE ANGLE
C14  AZIMUTH AT TANGENT POINT ALL IN DEGREES
C14
   0.104065E+03   0.000000E+00   0.281306E+02   0.000000E+00
C15 SOURCE-OBSERVER RANGE IN KM AND SHORT-LONG PATH INDEX
C15
  0.324247E+04      1
CNOTE ALL COMMENTS BELOW THIS INPUT PARAMETER WILL BE NEW
CNOTE  EACH TIME SHARC RUNS.  THEREFORE ANY COMMENTS THE USER
CNOTE  TO ADD TO THIS INPUT FILE SHOULD BE ABOVE THIS PARAMETER
CNOTE
C16 NUMBER OF REGIONS
C16
   1
C*1 REGION NUMBER AND REGION TYPE (0=AMBIENT,1=AURORAL)
C*1
   1   0
C*2 ATMOSPHERE MODEL FILE NAME
C*2
  NIG76.DAT
C*3 MONTE CARLO PARAMETERS : NUMBER OF PHOTONS,
C*3  MAXIMUM ORDER OF SCATTERING, SUNSHINE (1=YES,0=NO) AND
C*3  EARTHSHINE (1=YES,0=NO) INDICES
C*3
   20000      200       0       1
C1*1 POPULATION FILE NAME AND SAVE INDEX FOR ENVIRONMENT ONE
C1*1
  NIGHT.POP                         1
C1*2 NUMBER OF RADIATORS IN ENVIRONMENT ONE
```

```
C1*2
   2
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  CO2          1      0.984E+00
C-2 SPECIES LINKING FILE
C-2
  CO21LINK.REV
C-3 SPECIES STATES FILE
C-3
  CO21STAT.DAT
C-4 SPECIES BANDS FILE
C-4
  CO21BAND.DAT
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  NO           1      0.100E+01
C-2 SPECIES LINKING FILE
C-2
  NOLINK.REV
C-3 SPECIES STATES FILE
C-3
  NOSTAT.DAT
C-4 SPECIES BANDS FILE
C-4
  NOBAND.DAT
C17 MAXIMUM FREQUENCY, MINIMUM FREQUENCY AND RESOLUTION (1/cm)
C17
  0.300000E+04    0.400000E+04    0.100000E+01
C18 NUMBER OF SPECIES FOR RADIANCE CALCULATION
C18
     2
CR-01 MOLECULAR FORMULA AND ISOTOPE NUMBER
CR-01
    CO2       1
CR-01 MOLECULAR FORMULA AND ISOTOPE NUMBER
CR-01
    NO        1
```

TABLE 12. UPDATED SHARC.INP FILE.

```
C0 STANDARD INPUT FILE SHARC.INP
C0 THIS FILE HOLDS THE DEFAULT VALUES FOR SHARC
C0 THIS FILE IS UPDATED TO THE CURRENT VALUES OF THE PARAMETERS
C0 EACH TIME SHARC IS RUN.
C0 LINES WHICH HAVE A "C" IN COLUMN 1 ARE TREATED AS COMMENT
C0
C1 THE FIRST LINE CONTAINS THE INTERACTIVE/BATCH OPTION
C1 IF IT EQUALS 1, SHARC WILL RUN INTERACTIVELY, ALLOWING
C1 THE USER TO UPDATE OPTIONS.  IF IT EQUALS 0, SHARC WILL
C1 RUN IN BATCH MODE.
C1
   1
C2 TITLE FOR CALCULATION
C2
  NEW Title
C3 OUTPUT CONTROL PARAMETERS:
C3 1) MODEL ATMOSPHERE OUTPUT ==>1 FOR FULL LISTING
C3 2) SELECTED TRANSITIONS ==>1 FOR TRANSITIONS SELECTED
C3 3) MOLECULAR BAND INFORMATION ==>1 FOR BAND INFORMATION
C3 4) NOT CURRENTLY USED
C3 5) NEMESIS OUTPUT ==>1 NEMESIS ONLY ==>2 FOR POST POPULATIONS
C3 6) AURORAL OUTPUT ==>1 FINAL ONLY ==>2 TIME DEVELOPMENT
C3 7) FINAL STATE POPULATIONS ==>1 YES
C3 8) FINAL VIBRATIONAL TEMPERATURES ==>1 YES
C3 9) LOS OUTPUT ==>1 FOR COLUMN DENSITIES
C3 10)SPECTRAL RADIANCE OUTPUT ==>1 FOR RADIANCE OUTPUT
C3 1   2   3   4   5   6   7   8   9  10
   1   1   0   0   0   1   1   1   1   0
C4 FILE NAME (AND PATH) FOR SHARC LINE FILE
C4
  SHARC.LIN
C5 FILE NAME (AND PATH) FOR SHARC SPECTRAL RADIANCE OUTPUT FILE
C5
  SHARC.SPC
C6 FILE NAME (AND PATH) FOR SHARC TRANSMISSION OUTPUT FILE
C6
  SHARC.TRN
C7 FILE NAME (AND PATH) FOR SHARC GENERAL OUTPUT FILE NAME
C7
  SHARCNIGHT.OUT
C8 SOLAR ZENITH ANGLE IN DEGREES
```

```
C3
  0.100000E+02
C9 LINE-OF-SIGHT INFORMATION : PATH TYPE, CASE, ORIGIN LOCATION
C9 AND SPHERICAL EARTH INDEX
C9
   4     1     0     0
C10 OBSERVER INFORMATION: ALTITUDE (KM), LONGITUDE AND LATITUDE
C10
  0.300000E+03    0.000000E+00   -0.147555E+02
C11 SOURCE INFORMATION: ALTITUDE (KM), LONGITUDE AND LATITUDE
C11
  0.300000E+03    0.000000E+00    0.147555E+02
C12 TANGENT ALTITUDE, LONGITUDE AND LATITUDE AT TANGENT POINT
C12
  0.800000E+02    0.000000E+00    0.000000E+00
C13 LOS CASE INDEX, LONGITUDE AND LATITUDE ALONG LOS VECTOR
C13
     0  0.000000E+00  0.000000E+00
C14 ZENITH ANGLE, AZIMUTH ANGLE, OBSERVER-EARTH-SOURCE ANGLE
C14  AZIMUTH AT TANGENT POINT ALL IN DEGREES
C14
   0.104756E+03   0.000000E+00   0.295110E+02   0.000000E+00
C15 SOURCE-OBSERVER RANGE IN KM AND SHORT-LONG PATH INDEX
C15
  0.339814E+04      1
CNOTE ALL COMMENTS BELOW THIS INPUT PARAMETER WILL BE NEW
CNOTE  EACH TIME SHARC RUNS.  THEREFORE ANY COMMENTS THE USER
CNOTE  TO ADD TO THIS INPUT FILE SHOULD BE ABOVE THIS PARAMETER
CNOTE
C16 NUMBER OF REGIONS
C16
   2
C*1 REGION NUMBER AND REGION TYPE (0=AMBIENT,1=AURORAL)
C*1
   1   0
C*2 ATMOSPHERE MODEL FILE NAME
C*2
  NIG76.DAT
C*3 MONTE CARLO PARAMETERS : NUMBER OF PHOTONS,
C*3  MAXIMUM ORDER OF SCATTERING, SUNSHINE (1=YES,0=NO) AND
C*3  EARTHSHINE (1=YES,0=NO) INDICES
C*3
   20000      200        0        1
C1*1 POPULATION FILE NAME AND SAVE INDEX FOR ENVIRONMENT ONE
C1*1
  NIGHT.POP                       1
```

```
C1*2 NUMBER OF RADIATORS IN ENVIRONMENT ONE
C1*2
   2
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  CO2          1     0.984E+00
C-2 SPECIES LINKING FILE
C-2
  CO21LINK.REV
C-3 SPECIES STATES FILE
C-3
  CO21STAT.DAT
C-4 SPECIES BANDS FILE
C-4
  CO21BAND.DAT
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  NO           1     0.100E+01
C-2 SPECIES LINKING FILE
C-2
  NOLINK.REV
C-3 SPECIES STATES FILE
C-3
  NOSTAT.DAT
C-4 SPECIES BANDS FILE
C-4
  NOBAND.DAT
C*1 REGION NUMBER AND REGION TYPE (0=AMBIENT,1=AURORAL)
C*1
   2   1
C*2 ATMOSPHERE MODEL FILE NAME
C*2
  NIG76.DAT
C*3 MONTE CARLO PARAMETERS : NUMBER OF PHOTONS,
C*3  MAXIMUM ORDER OF SCATTERING, SUNSHINE (1=YES,0=NO) AND
C*3  EARTHSHINE (1=YES,0=NO) INDICES
C*3
   20000    200       0       0
C1*1 POPULATION FILE NAME AND SAVE INDEX FOR ENVIRONMENT ONE
C1*1
  NIGHT.POP                         2
C1*2 NUMBER OF RADIATORS IN ENVIRONMENT ONE
C1*2
   2
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
```

```
  NO            1      0.100E+01
C-2 SPECIES LINKING FILE
C-2
  NOLINK.DAT
C-3 SPECIES STATES FILE
C-3
  NOSTAT.DAT
C-4 SPECIES BANDS FILE
C-4
  NOBAND.DAT
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  CO2           1      0.984E+00
C-2 SPECIES LINKING FILE
C-2
  CO21LINK.DAT
C-3 SPECIES STATES FILE
C-3
  CO21STAT.DAT
C-4 SPECIES BANDS FILE
C-4
  CO21BAND.DAT
C2*1 POPULATION FILE NAME AND SAVE INDEX FOR ENVIRONMENT TWO
C2*1
  ANIGHT.POP                        1
C2*2 NUMBER OF RADIATORS IN ENVIRONMENT TWO
C2*2
   2
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  NO            1      0.100E+01
C-2 SPECIES LINKING FILE
C-2
  ANOLINK.DAT
C-3 SPECIES STATES FILE
C-3
  ANOSTAT.DAT
C-1 MOLECULAR FORMULA FOR SPECIES
C-1
  NO+           1      0.100E+01
C-2 SPECIES LINKING FILE
C-2
  ANO+LINK.DAT
C-3 SPECIES STATES FILE
C-3
  ANO+STAT.DAT
```

```
C#1 USER OR CODE DEFINED AURORAL INDEX
C#1
   1
C#2 AURORAL IBC INDEX
C#2
   3
C#3 DISTRIBUTION INDEX, TOTAL ENERGY, CHARACTERISTIC ENERGY,
C#3  AND SCALE PARAMETER
C#3
   1   0.10000E+03   0.50000E+01   0.00000E+00
C#4 DOSE TIME AND OBSERVATION TIME (SEC)
C#4
   0.10000E+03   0.10000E+03
C*4 ORIGIN OF COORDINATE SYSTEM INDEX
C*4
   0
C*5 FOUR LATITUDES FOR LOCAL REGION CORNERS (DEGREES)
C*5
   0.50000E+01   0.50000E+01  -0.50000E+01  -0.50000E+01
C*6 FOUR LONGITUDES FOR LOCAL REGION CORNERS (DEGREES)
C*6
   0.50000E+01   0.35500E+03   0.35500E+03   0.50000E+01
C*7 UPPER AND LOWER ALTITUDES OF LOCAL REGION (KM)
C*7
   0.12000E+03   0.80000E+02
C17 MAXIMUM FREQUENCY, MINIMUM FREQUENCY AND RESOLUTION (1/cm)
C17
  0.250000E+03   0.500000E+04    0.200000E+01
C18 NUMBER OF SPECIES FOR RADIANCE CALCULATION
C18
     3
CR-01 MOLECULAR FORMULA AND ISOTOPE NUMBER
CR-01
    NO       1
CR-01 MOLECULAR FORMULA AND ISOTOPE NUMBER
CR-01
    NO+      1
CR-01 MOLECULAR FORMULA AND ISOTOPE NUMBER
CR-01
    CO2      1
```

4.3 Detailed Parameter Discussion

This section defines the input parameters for the ambient and auroral populations, GEOMETRY, and SPCRAD modules. The Monte Carlo control parameters used in the ambient populations module warrant further description since their values effect the accuracy of the Monte Carlo simulation. Parameters used to define the auroral conditions are discussed in detail. The Geometry parameters section will describe the various subsets of geometry variables needed to define a LOS. Finally the parameters used to define the spectral interval, resolution and species included in the calculation are discussed.

4.3.1 Ambient Population Parameters

The ambient populations module contains a set of routines which determine the enhancement of the atmospheric excited states layer populations due to layer *radiative self-trapping* and layer-layer radiative pumping. The first-order population enhancement is determined using a Monte Carlo simulation of the initial source photon emission and absorption or escape. The number of photons determines the statistical uncertainty of the Monte Carlo calculation. Changing this variable to a small number saves computer time, but causes large statistical uncertainties. For reasonable statistical uncertainties the number of photons should be 20,000 or larger.

The maximum order of scattering parameter determines the number of matrix multiplications used by NEMESIS to calculate the population enhancement matrix. Changing this number to less than 100 does not save much computer time since the Monte Carlo simulation is performed for first-order scattering only and higher order scattering is determined recursively. Many orders of scattering may be important for some molecular

bands, such as 4.3 μm CO_2 radiation. A value of 200 for the maximum order of scattering is sufficiently large.

The remaining two parameters parameters turn on/off solar and earthshine pumping. A value of 1 means the pumping is on, and a value of 0 means the pumping is off.

4.3.2 Auroral Population Parameters

The model parameters describing an auroral event allows the user to either select a code supplied aurora or to define a user specified aurora, as well as specify the duration of the aurora and observation time. As employed in AARC[2], two simple forms for the auroral primary electron spectral flux are available in SHARC, a Maxwellian flux and a Gaussian flux. The Maxwellian flux is representative of diffuse auroras and is characterized by two parameters, the total energy flux and a characteristic energy (equal to one half the mean energy). The Gaussian flux is characteristic of electron energy spectra in discrete auroras, and is defined by three parameters, the total energy flux, the mean energy, and the energy variance. However, the user can select three typical auroral electron spectra with a Maxwellian distribution corresponding to IBC II, III, or III^+. Finally, the user must select the duration of the aurora, and the observation time relative to the beginning of the dosing (which is assumed to be 0). (The input units are: flux in $ergs/cm^2/sec$, energy in KeV, and time in sec.)

4.3.3 Geometry Parameters

The LOS is defined as the straight line which connects the observer located at a point H1 to the source located at H2. Curvature of the LOS due to refraction is negligible over the altitude regime considered in SHARC. Three classes of LOS paths are supported by SHARC and are specified through the variable IPATH:

IPATH = 2 -- observer to source,
= 3 -- observer to space, and
= 4 -- limb viewing.

The nomenclature used in the geometry module is derived from the low-altitude radiance code LOWTRAN 6.[8] In the current SHARC version, there is no IPATH = 1 option. There are a number of geometric parameters that must be specified in order to define each type of path, and these are defined in Table 13 and illustrated in Figure 3. Altitudes and ranges are given in km, and angles in degrees. Longitudes can have values ranging form 0^o to 360^o, and latitudes, from -90^o at the south pole to 90^o at the north pole. A0 is the local zenith angle of the LOS as measured from the vertical line connecting H1 and the earth center. The angle B0 is the azimuth of the LOS as measured in the plane normal to the vertical at the same altitude as the observer (e.g., the local horizontal); it varies from -180^o to 180^o.

TABLE 13. LOS PARAMETERS.

H1ALT	observer altitude
H1LONG	" longitude
H1LAT	" latitude
H2ALT	source altitude
H2LONG	" longitude
H2LAT	" latitude
HMIN	tangent height from the surface of the earth;
HMLONG	" point longitude
HMLAT	" point latitude
HPLONG	longitude of point along LOS vector
HPLAT	latitude of point along LOS vector
RANGE	distance from H1 to H2
BETA	earth-center angle between H1 and H2
A0	zenith angle of LOS at observer
B0	LOS azimuthal angle; north = 0 & east = 90^o
LEN	designates short or long paths for certain down-looking geometries

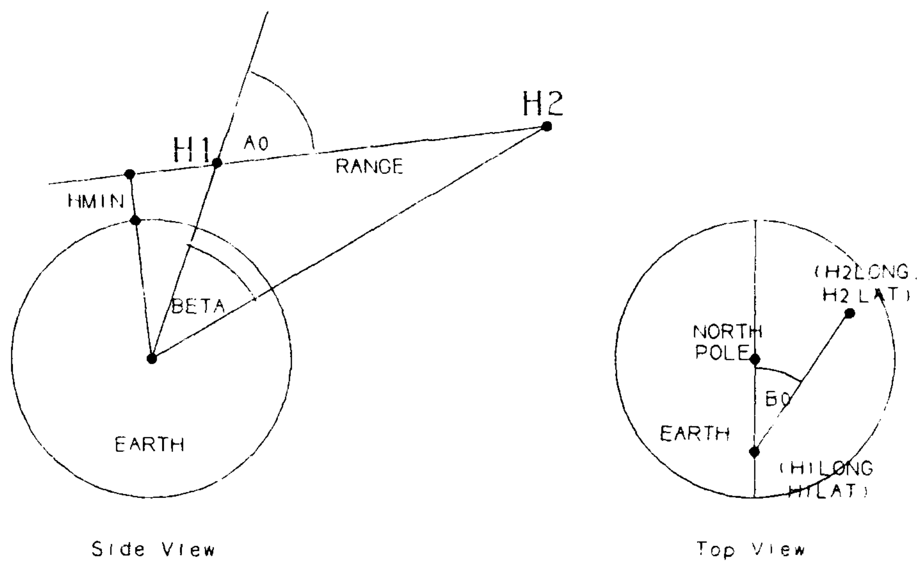


Figure 3. Definitions of LOS Parameters.

The parameters listed in Table 13 overspecify the LOS. For a particular LOS only one of many different subsets is required as input. The other parameters are calculated internally. Each class, designated by its IPATH value, has various options for specifying the LOS. These are labeled by the integer variable ICASE and are listed in Table 14 along with the required geometrical inputs. The particular case with IPATH = 2 and ICASE = 1 is ambiguous when H1 > H2. The two paths are distinguished with the LEN variable and are illustrated in Figure 4.

TABLE 14. GEOMETRY INPUT SEQUENCES.

IPATH	ICASE	Geometrical Inputs
2	1	H1, H2ALT, AO, BO*
		H1, H2ALT, AO, BO*, LEN
	2	H1, RANGE, AO, BO*
	3	H1, H2ALT, RANGE, BO*
	4	H1, H2ALT, BETA, BO*
	5	H1, H2ALT, H2LONG, H2LAT
3	1	H1, AO, BO*
	2	H1, HMIN, BO*
4	1	HMIN, HMLONG, HMLAT, BO*

Note: 1. H1 stands for (H1ALT, H1LAT, H1LONG).

2. * there are three ways to input the azimuth angle information:
(1) direct entry in degrees,
(2) defining a point along the LOS trajectory before HMIN, and
(3) defining a point along the LOS trajectory after HMIN.

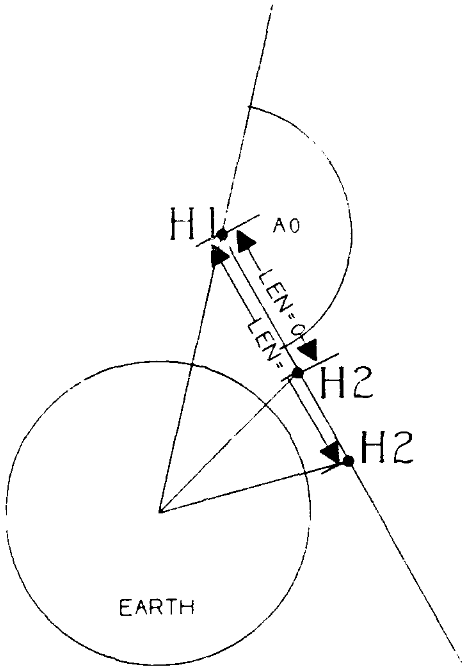


Figure 4. Specification of the LEN Parameter for Down-Looking Paths.

4.3.4 Spectral Radiance Parameters

The spectral range is defined by inputting the minimum and maximum frequency (cm^{-1}) of interest. SHARC currently includes lines from 250 to 10000 cm^{-1}. The spectral resolution is given in cm^{-1} and is currently limited to 0.1 cm^{-1}. The spectral radiance array can contain 10,000 points. So, if a 0.1 resolution is used only a 1000 cm^{-1} spectral range can be used. The interactive input module will alert the user if the range is too large for the selected resolution, and it will reset maximum frequency to reduce the range.

The user must specify the species desired for the radiance calculation. The list may be equal to, or a subset of the species

contained in population calculations or population files. The species are entered through the interactive input module by typing in their chemical formulas. Currently, only the major isotope of each species is represented, except for CO_2 which has eight isotopes in the menu. Three of these isotopes are currently supported with data files. The other five isotopes can be incorporated by developing the required data files following the discussion in Section 3. At the end of a calculation the total number of lines and the total number of relayered lines are summarized for each band and species in the general SHARC output file.

5. SHARC OUTPUT FILES

5.1 Error File

The SHARC error file (SHARC.ERR) contains error and warning statements generated during SHARC execution. The majority of error messages are due to improper preparation of the input files. Warning or caution messages usually result from inconsistent use of input files. An error message during execution is considered fatal, and execution will stop after the error message is written to the error file. A warning or caution message is not fatal (i.e., does not terminate execution), but it should inform the user that input files are inconsistent, that only a partial calculation has been performed, or that numerical difficulties have been encountered and fixed in one of the SHARC modules. The user should monitor the error file after each SHARC run to insure that the desired calculation was properly performed.

There are over 150 different error/caution messages which can be written to the error file during execution. The error/caution messages contain the subroutine name in which the problem occurred. As an example of an error message, consider an error resulting from inconsistent input in the molecular states (see Section 3.2) and bands (see Section 3.3) files. Assume that the 2→1 vibrational transition for CO has been specified in the molecular states file (see Table 5). If the data for the line strength distribution function for the 2→1 transition has not been included in the molecular bands file (see Table 6), the following error message will be written to the error file:

```
ERROR IN BANDIN...
     CO(1)      - CO(0)      BAND MISSING FROM BAND DATA prompting the
```

user to check the CO bands file for an input error or omission of data.

As seen in the previous example, the error/caution messages generated from input files are usually self-explanatory, and the user should be able to easily correct the problem. In some cases, however, the problem may be more subtle. For example, error/caution messages generated during calculation of number densities of vibrationally excited states most likely will require the user to carefully check the chemical kinetics mechanism and the list of transitions considered by ambient populations module.

5.2 General Output File

The general SHARC output file contains a summary of selected output from each module. As mentioned previously, there are three levels of output which can be obtained from each SHARC module. The level (and amount) of output is selected through the interactive menu (see Section 4.2). The level of output can be selected independently for several of the SHARC modules. The lowest level contains the minimum amount of information (IWRITE=0) necessary to characterize the calculation, and the highest level contains the maximum amount of information (IWRITE=2). The type of output which is written to the output file for the specified IWRITE option is illustrated in Table 15. Notice that the atmosphere name and the band radiance summary (see Table 15) are always written to the output file, and the spectral radiance as a function of frequency is always written to the plot file (see Section 5.4).

TABLE 15. TYPE OF OUTPUT CONTAINED IN SHARC.OUT FILE.

OUTPUT	OPTION	DESCRIPTION
Model Atmosphere	0	Atmosphere File Name
	1,2	Complete Atmosphere Input File
Selected Transitions	0	No Output
	1,2	Complete Molecular States Input File
Molecular Band Data	0,1	No Output
	2	Complete Molecular Bands Input File
Ambient Output	0	No Output
	1	Initial Steady State Layer Source Populations and NEMESIS Excited State Population Enhancements; Earthshine, Sunshine, and Atmospheric Excitation Rates; and the quenching/re-emission Probabilities
	2	Post NEMESIS Excited State Populations for Each Selected Transition
Auroral Output	0	No Output
	1	Final Population for all auroral species
	2	Populations of all auroral species as a function of time
Final Excited State Populations	0	No Output
	1,2	Final Excited State Populations
Final Excited State Temperatures	0	No Output
	1,2	Final Excited State Temperatures
Line of Sight Output	0	
	1,2	Species Total Column Densities Along Line of Sight
Spectral Radiance Output	0	Plot File (SHARC.SPC)
	1,2	Spectral Radiance Table

5.3 Population File

The excited-state populations for each atmospheric layer will change only when a new model atmosphere is used, day and night conditions change, a new solar zenith angle is defined or auroral conditions change. Thus, the excited-state populations and the information necessary to uniquely characterize them are written to a binary "population" file. This allows the user to perform multiple SHARC calculations for any number of observer-source scenarios without re-calculating the populations each time. The relevant information written to the "population" file is:

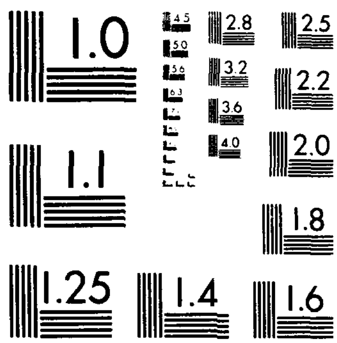
- The model atmosphere file (Section 3.5),
- The molecular radiators and the associated "linking", "states", and "bands" files,
- The list of species (Section 3.1) for each molecular radiator,
- The molecular states file (Section 3.2) for each molecular radiator,
- The excited state populations and associated temperatures for each molecular radiator, and
- The auroral parameters when auroral option is used.

For subsequent calculations using the "population" files, it is necessary to change only the input and output parameters relevant to the GEOMETRY and/or SPCRAD sections of the SHARC.INP file (Section 4.2-4.3). Although the complete set of options described in Section 5.2 for creating the general output file are not available when using a previously created "population" file, the output file does contains sufficient detail to uniquely characterize the "population" file used. However, the user should refer back to the original general output file generated when the population file was created if any greater detail is desired.

AD-A237 089 DESCRIPTION OF THE STRATEGIC HIGH-ALTITUDE ATMOSPHERIC RADIATION CODE (SH (U) SPECTRAL SCIENCES INC BURLINGTON MA J W DUFF ET AL 27 NOV 90 SSI-TR-176 2/2

UNCLASSIFIED GL-TR-90-0315 F19628-87-C-0130 F/G 4/1 NL

END
FILMED
DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

5.4 Spectral File

An ASCII file is created to allow the user to either plot the calculated spectral radiance directly or to further reduce the data. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used by SHARC. The plot file contains the frequency (cm^{-1}) and the spectral radiance ($W/sr/cm^2/cm^{-1}$) written as an (x,y) ordered pair with one pair per line.

5.5 Transmittance File

An ASCII file is created to allow the user to either plot the calculated spectral transmittance directly or to further reduce the data. For example, the user may wish to apply a specific filter function to the transmittance or to convert to a set of units other than those used by SHARC. The plot file contains the frequency (cm^{-1}) and the transmittance written as an (x,y) ordered pair with one pair per line.

6. RUNNING THE PLOTTING PACKAGE

The plotting software is a separate package which can be used to plot the SHARC spectral output. The plotting program, which is a general x-y plotting package, is interactive and has two menus of options. First, the program queries the user for the input file name that is to be read and plotted. The default name for the file is SPEC.OUT. This is the name of the spectral output file generated by the SHARC program. The input file is a unformatted list of x,y pairs without any header information. After the input file is read the menu options can be modified for a particular plotting case. The first menu has eight options which can be altered. These include the plot output file name, the titles for the plot and the x and y axes, the plot type, the location of the axis tic marks, and the lengths of the x and y axes. A set of standard default values of these parameters is presented to the user. These default values can be changed or the next menu can be accessed by typing a zero. The second menu allows the dynamic range of the radiance (y axis) and the wavenumber interval (x axis) to be adjusted. Default values are calculated from the input data file which span the entire dynamic range of the radiance and the entire wavenumber interval of the input. Adjustment of the number of major and minor tics on the axis is also an option of the second menu. A session with the plot package is included here to illustrate the interactive nature of the program. User responses are contained in brackets {..} to distinguish them from the program queries. Comments about the program queries and user responses are contained in the brackets <..>.

Begin session:

{run plot}

<An interactive session for plotting a SHARC output >
<spectrum. >

```
     THE DEFAULT FILE NAME IS SPEC.OUT
     IS THIS THE FILE YOU WANT PLOTTED? [Y,N]
{N}
           <Responding with a "n" causes the program to request an    >
           <input file.                                                >

     INPUT THE FILE NAME FOR THE DATA TO BE PLOTTED
{NOSPEC.OUT}
           <The program will now read in data from the disk file      >
           <file NOSPEC.OUT.                                           >

           <The first menu will now be printed on the screen.  Each   >
           <time it is presented it contains the current options.     >
           <Initially it contains default options.  When the          >
           <user is satisfied with the options, a "0" response        >
           <will cause the program to go to the next menu.            >

     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :OUTPUT.PLT
     2. Plot title       :SHARC SPECTRUM
     3. X-axis label     :WAVENUMBER
     4. Y-axis label     :RADIANCE
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{1}
           <Responding with a "1" causes the program to request a     >
           <new file name for the plot data.                          >


     INPUT THE NAME OF THE PLOT OUTPUT FILE
{NO.PLT}
           <The output plot data will be in file NO.PLT.              >


     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :SHARC SPECTRUM
     3. X-axis label     :WAVENUMBER
     4. Y-axis label     :RADIANCE
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
```

```
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{2}
           <Responding with a "2" causes the program to request a new  >
           <title for the plot.                                        >

     INPUT THE PLOT TITLE
{NO 60 km limb}
           <The plot title will now be "NO 60 km limb"                 >

     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :WAVENUMBER
     4. Y-axis label     :RADIANCE
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{3}
           <Responding with a "3" causes the program to request a new  >
           <label for the x axis.                                      >

     INPUT THE X-AXIS LABEL
{wavenumber (cm^-^1)}
           <The label will now be in lower case and contain units.     >


     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :RADIANCE
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{4}
           <Responding with a "4" causes the program to request a new  >
           <label for the y axis.                                      >
```

```
     INPUT THE Y-AXIS LABEL
{Spectral Radiance (W/sr/cm^2/cm^-^1}
           <The label will now be contain units.                          >

     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :Spectral Radiance (W/sr/cm^2/cm^-^1)
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{5}
           <Responding with a "5" causes the program to list its          >
           <plot type options and request a selection.                    >
     PLOT TYPES ARE:
     1 - LINEAR PLOT
     2 - SEMI-LOG PLOT (Y LINEAR)
     3 - SEMI-LOG PLOT (X LINEAR)
     4 - LOG-LOG PLOT

     INPUT YOUR CHOICE
{3}
           <Selecting plot type "3" causes the program to keep its        >
           <default semi-log radiance (wavenumber linear) form.           >

     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :Spectral Radiance (W/sr/cm^2/cm^-^1)
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :OUTSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{6}
           <Responding with a "6" causes the program to list its tic      >
           <mark options and request a selection.                         >

     TIC MARK TYPES ARE:
```

```
     1 - INSIDE GRAPH AXES
     2 - OUTSIDE GRAPH AXES

     INPUT YOUR CHOICE FOR TIC MARK DIRECTION
{1}
           <The tic marks will now be on the inside of the plot.       >

THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :Spectral Radiance (W/sr/cm^2/cm^-^1)
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :INSIDE GRAPH
     7. X-axis length in inches: 5.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{7}
           <Responding with a "7" causes the program to request a new  >
           <length for the x axis.                                     >

     INPUT THE X-AXIS LENGTH IN INCHES
{4.0}
           <The x axis will be four inches long.                       >
     THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :Spectral Radiance (W/sr/cm^2/cm^-^1)
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :INSIDE GRAPH
     7. X-axis length in inches: 4.0
     8. Y-axis length in inches: 5.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{7}
           <Responding with a "7" causes the program to request a new  >
           <length for the y axis.                                     >

     INPUT THE Y-AXIS LENGTH IN INCHES
{4.0}
           <The y axis will be four inches long.                       >


THE FOLLOWING VARIABLES HAVE BEEN SELECTED:
```

```
     1. Plot output file :NO.PLT
     2. Plot title       :NO 60 km limb
     3. X-axis label     :wavenumber (cm^-^1)
     4. Y-axis label     :Spectral Radiance (W/sr/cm^2/cm^-^1)
     5. Plot type        :SEMI-LOG PLOT (X LINEAR)
     6. Tic marks        :INSIDE GRAPH
     7. X-axis length in inches: 4.0
     8. Y-axis length in inches: 4.0

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{0}
           <Free at last.  By responding with a "0" ,the program       >
           <proceeds to the next menu.                                 >

           <The second menu has as defaults the dynamic ranges of      >
           <the x (frequency) and y (radiance) axes.  If only a        >
           <portion of the data is desired for the current plot the    >
           <options 1 and/or 2 should be selected.  The program tries  >
           <to adjust the ranges so that rounded numbers will be       >
           <selected for the tic marks.                                >

     THE FOLLOWING CHARACTERISTICS ARE SET FOR THE CURRENT PLOT:
     1. Minimum frequency          : 1500.0
     1. Maximum frequency          : 4500.049804
     2. Minimum radiance           : 9.999995E-21
     2. Maximum radiance           : 1.000001E-08
     3. Delta x between major ticks: 500.0
     4. Number of minor x ticks    : 4

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{1}
           <Responding with a "1" causes the program to request new    >
           <lower and upper limits of x (frequency).                   >

     INPUT X-MIN OR MINIMUM FREQUENCY FOR PLOT
{1600}

     INPUT X-MAX OR MAXIMUM FREQUENCY FOR PLOT
{2200}

     THE FOLLOWING CHARACTERISTICS ARE SET FOR THE CURRENT PLOT:
     1. Minimum frequency          : 1600.0
     1. Maximum frequency          : 2200.020019
     2. Minimum radiance           : 9.999995E-21
     2. Maximum radiance           : 1.000001E-08
     3. Delta x between major ticks: 500.0
```

```
     4. Number of minor x ticks     : 4

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{2}
           <Responding with a "2" causes the program to request new      >
           <lower and upper limits of y (radiance).                      >

     INPUT Y-MIN OR MINIMUM RADIANCE FOR PLOT
{1e-14}

     INPUT Y-MAX OR MAXIMUM RADIANCE FOR PLOT
{1e-8}

     THE FOLLOWING CHARACTERISTICS ARE SET FOR THE CURRENT PLOT:
     1. Minimum frequency           : 1600.0
     1. Maximum frequency           : 2200.020019
     2. Minimum radiance            : 9.999993E-15
     2. Maximum radiance            : 1.000001E-08
     3. Delta x between major ticks: 500.0
     4. Number of minor x ticks     : 4

     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{3}
           <Responding with a "3" causes the program to request a        >
           <new delta x (frequency interval) between major tics.         >

     INPUT DELTA X BETWEEN MAJOR TICKS
{200}
           <There will be 200 cm^-^1 between major tics.                 >

     THE FOLLOWING CHARACTERISTICS ARE SET FOR THE CURRENT PLOT:
     1. Minimum frequency           : 1600.0
     1. Maximum frequency           : 2200.020019
     2. Minimum radiance            : 9.999993E-15
     2. Maximum radiance            : 1.000001E-08
     3. Delta x between major ticks: 200.0
     4. Number of minor x ticks     : 4
     INPUT ITEM NUMBER TO BE CHANGED OR ZERO TO EXIT
{4}
           <Responding with a "4" causes the program to request a        >
           <new number of minor x ticks.                                 >

     INPUT NUMBER OF MINOR X TICKS
{3}
           <The number of minor tics has been changed to "3"             >
```

```
THE FOLLOWING CHARACTERISTICS ARE SET FOR THE CURFENT PLOT:
1. Minimum frequency          : 1600.0
1. Maximum frequency          : 2200.020019
2. Minimum radiance           : 9.999993E-15
2. Maximum radiance           : 1.000001E-08
3. Delta x between major ticks: 200.0
4. Number of minor x ticks    : 3

Input item number to be changed or zero to exit
{0}
      <Free at last. By responding with a "0" the data will be    >
      <plotted according to the current options.                  >
```

The result of the interactive session is that a file named NOSPEC.OUT is read from disk and a plot file named NO.PLT is generated with the labels and specifics generated during the terminal session. The resulting plot is presented in Figure 5.

The plot package allows superscripts, subscripts and Greek symbols to be used in the plot and axis labels. This is accomplished using key characters. Quotes, ", which surround the key characters in this text should not be typed at a terminal session.

|@ The symbol following a "^" will be plotted as a superscript.

|@ The symbol following a "\" will be plotted as a subscript.

|@ The symbol following a "|" will be replaced by a greek symbol according to Table 16.

|@ The symbol following a "#" will overwrite the previous symbol, that is a backspace will be performed prior to writing the symbol.

The above key characters can be plotted by preceding them with a "|". (i.e., "||" will result in a "|" being plotted, etc.)

TABLE 16. THE KEYS FOR GREEK LETTERS AND SPECIAL CHARACTERS.

KEY	GREEK LETTER	ASCII VALUE
0	CAPITAL GAMMA	48
1	CAPITAL DELTA	49
2	CAPITAL THETA	50
3	CAPITAL LAMBDA	51
4	CAPITAL PI	52
5	CAPITAL SIGMA	53
6	CAPITAL PHI	54
7	CAPITAL PSI	55
8	CAPITAL OMEGA	56
9	INFINITY	57
>	GREATER THAN OR EQUAL TO	62
A	LOWER CASE ALPHA	65
B	LOWER CASE BETA	66
C	LOWER CASE GAMMA	67
D	LOWER CASE DELTA	68
E	LOWER CASE EPSILON	69
F	LOWER CASE ZETA	70
G	LOWER CASE ETA	71
H	LOWER CASE THETA	72
I	DEL OPERATOR	73
K	SCRIPT 1	75
L	LOWER CASE LAMBDA	76
M	LOWER CASE MU	77
N	LOWER CASE NU	78
O	LOWER CASE XI	79
P	LOWER CASE PI	80
R	LOWER CASE RHO	82
S	LOWER CASE SIGMA	83
T	LOWER CASE TAU	84
U	LOWER CASE PHI	85
V	LOWER CASE PSI	86
W	LOWER CASE OMEGA	87
X	LOWER CASE CHI	88
Y	VECTOR HAT	89
[	RIGHT ARROW	91
]	LEFT ARROW	93

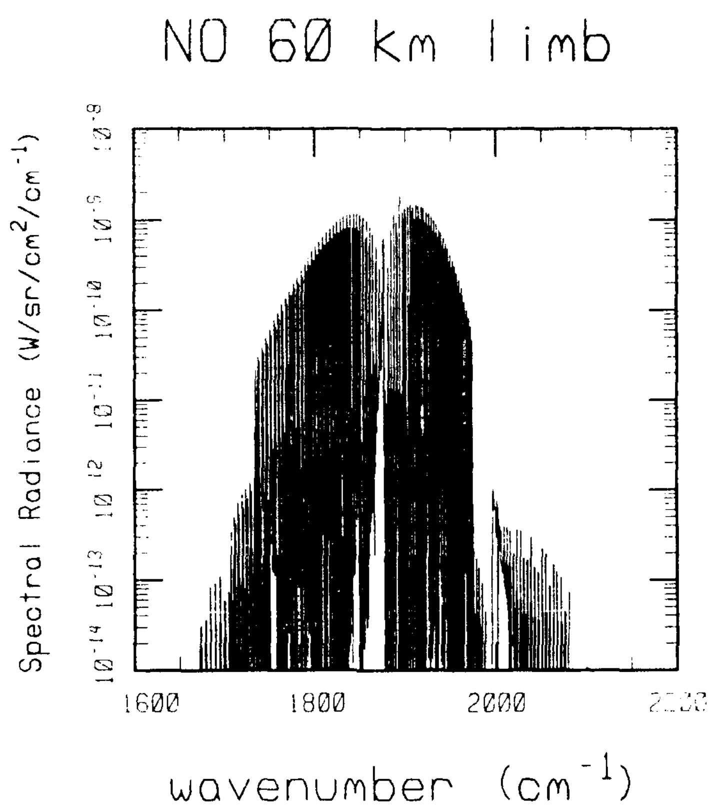


Figure 5. Sample NO Spectral Radiance Plot Created During Interactive Session.

7. REFERENCES

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APPENDIX A

IMPLEMENTATION INSTRUCTIONS

SHARC, version 2.0 of the Strategic High-Altitude Radiance Code, is furnished on a magnetic tape that contains the FORTRAN source code, input data sets and three test cases. The code calculates the spectral radiance from 250 to 5000 cm^{-1} for arbitrary geometries from 50 to 300 km. SHARC includes radiance from CO_2, H_2O, NO+, NO, O3, OH and CO.

The tape contains 69 files. There are a total of 13 FORTRAN files: ten for SHARC, one for the interpreter, one for the plotting package and one for the ASCII to binary conversion program. The others consist of four model atmosphere files, one generic input file, 24 input files for the eight current ambient molecular radiators, six input files for the auroral radiators, one ASCII line position and strength file, eleven interpreter output files, and input and output files from three test cases.

The tape format is:

9 track
1600 BPI
unlabeled ASCII
69 files
80 characters per record (files 1-49)
132 characters per record (files 50-69)
20 records per block.

The files are:

<u>SHARC-2 SOURCE CODE</u>

1	sharc	Main program	FORTRAN	547 lines
2	ambien	Ambient environment	FORTRAN	2046 lines
3	aurora	Auroral environment	FORTRAN	565 lines
4	chemkin	CHEMKIN subroutines	FORTRAN	3916 lines
5	geomtry	Geometry subroutines	FORTRAN	650 lines
6	input	Input subroutines	FORTRAN	2713 lines
7	intact	Interactive subroutines	FORTRAN	7933 lines
8	output	Output subroutines	FORTRAN	1355 lines
9	regvar	Region subroutines	FORTRAN	397 lines
10	spctra	Spectral Radiance subroutines	FORTRAN	781 lines

SUPPORTING SOURCE CODES				
11	interp	CHEMKIN Interpreter program	FORTRAN	2081 lines
12	pltpak	Plotting Package	FORTRAN	3609 lines
13	binary	Program to convert line data base to binary	FORTRAN	28 lines
MODEL ATMOSPHERES				
14	DAY76.DAT	1976 Standard Day	DATA	204 lines
15	NIG76.DAT	1976 Standard Night	DATA	204 lines
16	DAYSUBAR.DAT	Subarctic Summer Day	DATA	204 lines
17	NIGSUBAR.DAT	Subarctic Summer Night	DATA	204 lines
DEFAULT INPUT FILE				
18	SHARC.INP	Default Input File	DATA	186 lines
SPECIES DATA FILES				
19	CO21BAND.DAT	CO_2 Band Information file for 1st Isotope	DATA	594 lines
20	CO21KIN.DAT	CO_2 Kinetics file for 1st isotope	DATA	241 lines
21	CO21STAT.DAT	CO_2 Transitions and state file for 1st Isotope	DATA	65 lines
22	CO22BAND.DAT	CO_2 Band Information file for 2nd Isotope	DATA	470 lines
23	CO22KIN.DAT	CO_2 Kinetics file for 2nd isotope	DATA	241 lines
24	CO22STAT.DAT	CO_2 Transitions and state file for 2nd Isotope	DATA	65 lines
25	CO23BAND.DAT	CO_2 Band Information file for 3rd Isotope	DATA	405 lines
26	CO23KIN.DAT	CO_2 Kinetics file for 3rd isotope	DATA	241 lines
27	CO23STAT.DAT	CO_2 Transitions and state file for 3rd Isotope	DATA	65 lines
28	H2OBAND.DAT	H_2O Band Information file	DATA	217 lines
29	H2OKIN.DAT	H_2O Kinetics file	DATA	66 lines
30	H2OSTAT.DAT	H_2O Transitions and state file	DATA	27 lines
31	O3BAND.DAT	O_3 Band Information file	DATA	263 lines
32	O3KIN.DAT	O_3 Kinetics file	DATA	140 lines
33	O3STAT.DAT	O_3 Transitions and state file	DATA	46 lines
34	COBAND.DAT	CO Band Information file	DATA	41 lines
35	COKIN.DAT	CO Kinetics file	DATA	23 lines
36	COSTAT.DAT	CO Transitions and state file	DATA	11 lines
37	NOBAND.DAT	NO Band Information file	DATA	55 lines
38	NOKIN.DAT	NO Kinetics file	DATA	18 lines
39	NOSTAT.DAT	NO Transitions and state file	DATA	11 lines

SPECIES DATA FILES (cont.)

40	OHBAND.DAT	OH Band Information file	DATA	433 lines
41	OHKIN.DAT	OH Kinetics file	DATA	87 lines
42	OHSTAT.DAT	OH Transitions and state file	DATA	34 lines
43	ACO2KIN.DAT	CO_2 Auroral Kinetics file for 1st isotope	DATA	637 lines
44	ACO2STAT.DAT	CO_2 Auroral transitions and state file for 1st Isotope	DATA	26 lines
45	ANOKIN.DAT	NO Auroral Kinetics file	DATA	666 lines
46	ANOSTAT.DAT	NO Auroral Transitions and state file	DATA	41 lines
47	ANOPKIN.DAT	NO+ Auroral Kinetics file	DATA	625 lines
48	ANOP.DAT	NO+ Auroral Transitions and state file	DATA	32 lines

LINE DATA FILE

49	LINE.ASC	ASCII line parameter file	DATA	155190 lines

INTERPRETER OUTPUT

50	CO21OUT.DAT	CO_2 output for 1st isotope	DATA	339 lines
51	CO22OUT.DAT	CO_2 output for 2nd isotope	DATA	338 lines
52	CO23OUT.DAT	CO_2 output for 3rd isotope	DATA	338 lines
53	H2OOUT.DAT	H_2O output	DATA	106 lines
54	O3OUT.DAT	O_3 output	DATA	239 lines
55	COOUT.DAT	CO output	DATA	51 lines
56	NOOUT.DAT	NO output	DATA	42 lines
57	OHOUT.DAT	OH output	DATA	119 lines
58	ACO2OUT.DAT	CO_2 Auroral output	DATA	704 lines
59	ANOOUT.DAT	NO Auroral output	DATA	728 lines
60	ANOPOUT.DAT	NO+ Auroral output	DATA	688 lines

FIRST TEST CASE

61	SHARC1.INP	Test default file	DATA	186 lines
62	SHARC1.OUT	General output	DATA	2045 lines
63	SHARC1.SPC	Spectral file	DATA	3447 lines

SECOND TEST CASE

64	SHARC2.INP	Test default file	DATA	228 lines
65	SHARC2.OUT	General output	DATA	3002 lines
66	SHARC2.SPC	Spectral file	DATA	1488 lines

THIRD TEST CASE

67	SHARC3.INP	Test default file	DATA	141 lines
68	SHARC3.OUT	General output	DATA	1897 lines
69	SHARC3.SPC	Spectral file	DATA	970 lines

The FORTRAN source code for SHARC is found in the first ten files on the tape. These files should be compiled and linked to make the executable version. The only system-dependent routine is subroutine DATE which is in the input file (file six). This routine should return the date in a CHARACTER*32 variable called ADATE. All open statements for external files are in the main SHARC routine and the interactive menu module. The open statements may need to be changed for your machine. The SHARC subroutines are listed in Appendix C, and execution of SHARC is described in Section 4.

The INTERPRETER should be compiled as a stand-alone program. INTERPRETER subroutines are described in Appendix B, and use of the program is discussed in Section 4.

The plotting package should be compiled as a stand-alone program. The required system-dependent routines are discussed in Appendix D.

The routine called binary converts the ASCII line parameter file shipped on the tape to a binary form for SHARC. Binary should be compiled as a stand-alone program. When binary is executed it reads a file called LINE.ASC and outputs a binary version of the file. The new file is called SHARC.LIN. The conversion of LINE.ASC to SHARC.LIN is performed only once.

APPENDIX B

INTERPRETER SUBROUTINES

The INTERPRETER reads this symbolic description of an arbitrary chemical kinetics mechanism and translates it into the appropriate differential equations. The output from the INTERPRETER used by SHARC is a binary "linking" file which contains all the information describing the kinetic mechanism for a given molecular radiator.

A list of the subroutines comprising the INTERPRETER with a brief description follows.

<u>MAIN</u> MAIN opens the input and output files used by the INTERPRETER, and defines the following parameters used to set the maximum size of storage arrays:

KMX (=100)	The maximum number of species allowed during the execution of the INTERPRETER.
LENSYM(=10)	The maximum length of a species symbol.
MAXSP (=8)	The maximum number of species allowed in any given reaction.
MAXTB (=6)	The maximum number of third bodies allowed in any given reaction.
NRCOF (=4)	The number of parameters describing the reaction rate constant.
MXLEN (=80)	The maximum length of an input string.
MXLENR(=60)	The maximum length of a reaction input string.

<u>CKINTP</u> CKINTP is the driver routine which reads the species and reaction mechanism input, checks for proper syntax, and writes the "linking" file.

<u>CKTBD</u> This subroutine checks to make sure that different third-body efficiency factors have not been input for any species.

<u>CKINTC</u> This routine converts a character input string into internal code.

<u>CKNUM</u> CKNUM converts a character string into a specified number of real numbers. The character string may contain integer, floating point, or exponential numbers separated by at least one blank.

<u>CKSCAN</u> This subroutine scans a character string (in internal code) and converts all digits into integer numbers and all species into species indices.

<u>CKPARS</u> CKPARS checks the input string for format errors (i.e., enforce the rules given in Section 3.1)

<u>CKERR</u> This subroutine writes the error messages into the output file.

APPENDIX C

SHARC SUBROUTINES

A list of the subroutines comprising the various SHARC modules described in Section 2.2 is given below.

MAIN

The SHARC MAIN routine opens the input and output files used by SHARC, and calls: the input and output routines, the AMBIENT module, the AURORA module, the GEOMETRY module, and the SPCRAD module. MAIN also defines the following parameters used to determine the size of various arrays.

NAMLMX(=32)	The maximum number of characters for input/output file names.
NBINMX(=10000)	Maximum number of radiance bins.
NBMAX (=31)	Maximum number of bands.
NBYMAX(=66)	The maximum number of layer boundaries.
NCHMAX(=80)	Maximum length of reaction input string.
NDMAX (=400)	Maximum number of lines in the defaults file.
NEDGMX(=4)	
NENVMX(=2)	The maximum number of environments for each region.
NIMAX (=700)	The maximum number of reactions.
NISOMX(=8)	The maximum number of isotopes for each species.
NKMAX (=75)	The maximum number of species allowed.
NLNMAX(=10)	The maximum length of a species symbol.
NMMAX (=35)	The maximum number of atmospheric species.
NMOLMX(=7)	The maximum number of distinct radiating molecules.
NRDMX (=14)	Maximum number of molecular emitters.
NREGMX(=2)	Maximum number of regions.
NSECMX(=4)	
NSEGMX(=[illegible])	The maximum number of major segments along a line of sight.
NSMAX (=20)	The maximum number of bins for band distributions.
NSPMAX(=8)	The maximum number of species allowed in any given reaction.
NSTRMX(=72)	Maximum number of characters in a character string in the defaults file.
NTBMAX(=6)	The maximum number of third bodies allowed in any given reaction.
NTMPMX(=5)	The maximum number of temperatures for band distributions.
NVARMX(=20)	
NVMAX (=35)	The maximum number of vibrational states for each molecular emitter.
NWMAX(=200)	The maximum number of frequency bins for the Voigt line shape function.
[illegible]	The [illegible]

INTERACTIVE Module

ACTIVE — ACTIVE reads the first data line in the default file to determine if the calculation is interactive or batch.

ARCCOS — ARCCOS checks argument of arccosine to make sure it is between 1.0 and -1.0, then computes ACOS.

ARCSIN — ARCSIN checks argument of arcsine to make sure it is between 1.0 and -1.0, then computes ASIN.

ARCTAN — ARCTAN returns an angle between 0 and 2π given the end coordinates of a line with one vertex at the origin.

ADDRAD — ADDRAD is the input routine which is used to add radiative species to the ambient and auroral population calculations.

ADDREG — ADDREG is the routine for reviewing, editing and adding regional information.

AZI — AZI computes the local azimuth given the latitude of two points and the angle between them. ?

CHECKG — CHECKG checks the geometry inputs prior to an calculation.

CHKREG — CHKREG checks all regional information, such as filenames and input variable prior to an calculation.

CLNGTH — CLNGTH determines length of character string.

COMOUT — COMOUT prints standard comments into the defaults file.

CONDTR — CONDTR converts all angles to radians and transforms coordinates to geographic coordinates.

CONRTD — CONRTD converts all angles to degrees and transforms coordinates to magnetic north pole coordinates.

CROSS — CROSS takes the cross product between two vectors using the right hand rule.

DOT — DOT takes dot product of two vectors.

DFLTSG — DFLTSG reads the regional information found in the defaults file.

DUMPDE — DUMPDE writes the current values of the input variables into the defaults file.

FCHECK — FCHECK opens files and checks there status against the expected status. For example, does a new file already exist.

GEOMEX GEOMEX completes the full (over complete) set of variables which describe the line-of-sight.

INATM INATM is the interactive input routine for reviewing/changing the user's choice of model atmosphere.

INAUR INAUR is the interactive input routine for reviewing/changing the user's choice of auroral conditions.

INBOND INBOND is the interactive input routine for inputing the parameters which define a local region.

INGEOM INGEOM reads LOS geometry information from the default file and allows the user to review/change the parameters.

INMOL INMOL is the interactive input routine for reviewing/changing the radiators included in the population calculations.

INNAME INNAME is the interactive input routine for reviewing/changing the names for the standard input and output files.

INNEM INNEM is the interactive input routine for reviewing/changing the input parameters for the Monte Carlo radiation trapping module.

INOUT INOUT allows the user to review and/or modify the amount of output written to the general output file.

INPOP INPOP is the interactive input routine for reviewing/changing the population file names and status.

INREGN INREGN is the main interactive input routine for reviewing/changing regional information.

INSIDE INSIDE determines whether the local region forms a proper convex spherical pyramid.

INSOL INSOL is used to change/review the solar zenith angle.

INSPEC INSPEC is the interactive input routine used to change and/or modify the spectral range, resolution and species included in spectral radiance calculation.

INTITL INTITL is the interactive input routine for reviewing/changing the title of the calculation.

INTYPE INTYPE is the interactive input routine used to change the environment type. SHARC currently has two environments: ambient and auroral.

LATI — LATI computes the latitude of point "I" in radians given the latitude of another point, "II" and the latitude of point I to II.

LATPHI — LATPHI calculates the latitude and longitude of vector 2 relative to vector 1, given the latitudes and longitudes of vectors 1 and 2 relative to a common vector.

LONGI — LONGI computes the longitude of point "I" in radians given the longitude of another point, "II" and the longitude of point I to II.

LOADDE — LOADDE opens and loads the input data found in SHARC.INP into the array DFLTS. IF SHARC.INP this routine calls NODFTS to load in a set of default parameters.

LOS — LOS determines the line-of-sight vector.

MAJSEG — MAJSEG determines the major segments of the LOS through a region.

MCHECK — MCHECK checks the range of the variable to verify that the variable value is between the given bounds.

NODFTS — NODFTS loads the default values for a calculation into SHARC.INP when an SHARC.INP is not found.

NORM — NORM normalizes a 3 vector.

OPSANG — OPSANG computes the supplemental angle.

PARSEC — PARSEC separates text and numerical input parameters from an input character string.

PLSECT — PLSECT determines the intersection of a line-of-sight vector with a plane.

POLL — POLL contains the main interactive menu for running SHARC.

PROBDF — PROBDF is the main driver for the interactive menu or batch execution of SHARC. This routine determines all of the input parameters for a sharc calculation.

PYRINT — PYRINT computes the segment boundaries of the LOS that are within a spherical pyramid.

RADE — RADE computes the earth radius as a function of latitude.

RANGER — RANGER computes the over complete set of LOS geometry parameters.

RCHECK — RCHECK checks the range of the variable to verify that the variable value is between the given bounds.

REDCHR — REDCHR reads user response to queries which require character string answers.

REGANG — REGANG maps an arbitrary angle to a specified interval of 2 π.

REDINT — REDINT reads user response to queries which require integer answers.

REDREL — REDREL reads user response to queries which require real variable answers.

REGDTR — REGDTR converts edge latitudes and longitudes to radians and converts to geographic coordinates if necessary.

REGLOS — REGLOS determines if observer or source is inside the angular region.

RMRAD — RMRAD eliminates a radiator from the list of species desired for population calculation.

RMREG — RMREG is used to remove an unwanted region.

SETGEO — SETGEO initializes geometry parameters.

SPCCHK — SPCCHK checks to ensure that populations exist for all species selected for spectral calculation.

STUFFD — STUFFD fills dflts array with regional input information.

UNIVEC — UNIVEC determines the unit vector from latitude and longitude.

UPCASE — UPCASE converts a character string to all upper case characters.

VECPOL — VECPOL determines a cartesian vector from an altitude, latitude and longitude.

VECVRT — VECVRT determines polar coordinates from a cartesian vector.

INPUT Module

ATMDEN — This subroutine loads atmospheric profile into the appropriate local arrays.

ATMIN ATMIN identifies the atmospheric species in the general species list, and reads atmospheric profile (containing the species number densities and kinetic temperature).

ATMLYR ATMLYR computes the atmospheric properties for each layer.

ATMSYM ATMSYM sets up the character arrays identifying the atmospheric species and an indexing array which relates the atmospheric species to the species read by CKLINK.

BANDIN BANDIN reads the molecular bands file (Section 3.3), which describes the line strength distribution function parameters for each vibrational transition.

BLKDAT BLOCK DATA contains some fundamental constants, species molecular weights, the average atmospheric temperature for NEMESIS, and the optical depth cutoff parameter for the relayering option.

CKLINK CKLINK reads the "linking" file created by INTERP, and defines the arrays containing information on species names, chemical kinetics mechanism (i.e., the stoichiometric coefficients) and the rate constants.

DATE DATE calls a system-dependent routine to determine the date and time of the SHARC run.

RADIN This subroutine reads the molecular states file (Section 3.2), which contains the molecular radiator, the vibrational states included in the mechanism and the transitions to be considered by NEMESIS and SPCRAD.

RETREV This routine reads the saved population file data.

XNUM XNUM translates an alphanumeric character string containing N integer, real, or exponential numbers into their respective real values.

AMBIENT Module

AMBDRV This subroutine calls the appropriate CHMKIN/NEMESIS subroutines to compute the enhanced vibrationally excited state populations.

ARATE ARATE solves the two-state steady-state equation for the atmospheric excitation rate constant.

COLDEN COLDEN computes the total column density for each atmospheric layer for the radiating species.

CPF12 — CPF12 calculates the real part of the complex probability function for a Voigt line shape.

DEWV — DEWV computes the equivalent width for a single isolated Voigt line.

DWIDTH — DWIDTH calculates the Doppler halfwidth.

E2 — E2 computes the second exponential integral as a function of optical depth.

EMISS — This subroutine locates the Einstein A coefficient for the current transition, and also calculates the sum of all Einstein A coefficients for all transitions from the upper vibrational state.

ERATE — ERATE calculates the earthshine excitation rate for each atmospheric layer.

ESCPRB — ESCPRB normalizes the escape probabilities calculated by subroutine PATH for each layer.

ESHINE — ESHINE calculates the earthshine flux for the current transition using the specified effective earthshine temperature.

FORMV — FORMV calculates the Voigt line shape function.

LWIDTH — LWIDTH calculates the Lorentz halfwidth.

MULSCT — MULSCT calculates the nth-order multiple scattering enhancement to the excited-state number density using the single-scattering enhancement matrix.

NEMDRV — NEMDRV is the driver routine to compute the escape probabilities and enhanced excited-state number densities for each atmospheric layer using Monte Carlo integration of atmospheric layers, line strengths, and frequencies.

NEMFAC — NEMFAC computes the probability of escaping a specified layer and the excitation of the layer from all other layers. These quantities are used for the subsequent auroral calculation.

NEMRXN — NEMRXN identifies the excitation and relaxation processes in the chemical kinetics mechanism for the current transition being considered by NEMESIS.

PATH — PATH integrates through the atmospheric layers to determine the escape probabilities and single-scattering enhancements.

PICKSJ — PICKSJ determines the line strength selected from the line strength distribution function.

PICKZ — PICKZ finds the initial location and the corresponding layer for photon emission.

POPLTE — This subroutine computes the LTE populations for N_2 and O_2 which are subsequently used in the calculation of vibrationally excited states for CO and H_2O.

N2FAC — N2FAC computes the effective rate constant for the $CO_2(00011)$ + $N_2(0)$ quenching process and the excited state populations for N_2 following Kummer and James.

QUENCH — This subroutine computes the total quenching rate for the upper state of the transition.

RANF — This machine-dependent function generates uniformly distributed random numbers between 0 and 1.

SINTRP — SINTRP performs a linear interpolation to obtain the line strength distribution function for the appropriate layer temperature.

SOLAR — This subroutine calculates the solar flux at the transition frequency assuming a 5500 K blackbody.

SRATE — SRATE calculates the solar excitation rate for each atmospheric layer.

STEADY — STEADY sets up the steady state rate equations and then uses LUDCMP and LUBKSB to solve the set of linear algebraic equations for the number densities c_k. The major limitation to the steady-state procedure used here is the assumption that the rate equations are linear in the unknown vibrational population, i.e., there is no energy exchange among the emitting species. This restriction can be easily relaxed by using an algorithm which solves nonlinear equations (as opposed to LUDCMP/LUBKSB).

VOIGT — This subroutine determines the emission frequency using a Voigt line shape function. The absorption cross section at this frequency is also computed.

AURORAL Module

ALAM — ALAM computes Grun's universal energy-dissipation function using a linear interpolation of tabulated values.

AURDRV — AURDRV is the driver routine for the time-dependent auroral calculation. The auroral species number densities are returned to SHARC main at the observation time specified by the user.

CKLOAD CKLOAD loads the populations computed during the ambient calculation as the initial number densities for the auroral species.

EPFLUX EPFLUX calculates the primary energy flux assuming either a Gaussian or Maxwellian distribution function for the electron spectra.

IPPRAT IPPRAT calculates the ion pair production rate as a function of altitude for the specified auroral energy parameters.

RATMOD RATMOD modifies the Einstein A-coefficients and loads the layer excitation rates into the appropriate rate constant arrays. These quantities are computed by the ambient calculation.

RKLOAD RKLOAD transfers the layer-dependent rate constants into an array in order to interface with the numerical integration package.

TIMDEP TIMDEP controls the time dependent integration of the auroral rate equations.

CHEMKIN Module

ARATCON ARATCON uses the kinetic data from the auroral linking file to compute the rate constants as a function of temperature in exactly the same manner as RATCON (see below). However, ARATCON identifies primary electron processes and uses the input ionization efficiencies and the ion pair production rate to compute rate constants for secondary electron formation.

FUN FUN supplies LSODE with the species production rates obtained from PRAT.

JAC JAC supplies LSODE with the Jacobian of the species production rates obtained from PRATJ.

LUDCMP/LUBKSB

These two subroutines use a LU decomposition procedure to solve a set of simultaneous linearly independent algebraic equations (the steady-state equations).

PRAT PRAT uses the data obtained from the "linking" file to set up the differential equations for the species production rates.

PRATJ PRATJ uses the data obtained from the "linking" file to set up the Jacobian of the species production differential equations with respect to the species number densities.

RATCON This subroutine uses the kinetic data from the linking file to compute the rate constants as a function of temperature. The assumed form of the rate constant is

$$k = A\, T^{\beta} \exp(-E/T - C/T^{1/3}) \quad ,$$

where A is the pre-exponential factor, β is the exponent of the temperature term, E is the activation energy (can also be used to write a reverse rate constant in terms of the forward rate constant via detailed balance), and C is the (historic) SSH $T^{1/3}$ coefficient.

LSODE The LSODE package performs the numerical integration of the auroral rate equations. The package uses Gear's method for stiff differential equations and is supplied with the Sandia Livermore CHEMKIN code. The following subroutines/functions are used by the LSODE package: INTDY, STODE, CFODE, PREPJ, SOLSY, EWSET, VNORM, DGEFA, DGESL, DGBFA, DGBSL, DAXPY, DSCAL, DDOT, IDAMAX, DIMACH, XERRWV. For a brief description of these routines, see SUBROUTINE LSODE.

REGION Module

GVLOAD GVLOAD transfers the number densities, vibrational transitions, and related information from the regional arrays into global arrays, which are ultimately used by SPCRAD.

GVZERO GVZERO initializes all of the global variable arrays.

RVLOAD RVLOAD transfers the number densities, vibrational transitions, and related information from the local environment arrays into regional arrays.

RVZERO RVZERO initializes all of the regional variable arrays.

GEOMETRY Module

SEGGEN SEGGEN generates minor segments for each major segment along the specified line-of-sight.

SEGMNT SEGMNT computes major segment properties, including the major segment lengths, the number of major segments, and identifies the lower boundary for each segment.

PROCAL PROCAL calculates the line-of-sight properties for a major segment in a single region.

SPCRAD Module

BNDCMP This subroutine compares the transition listed on the HITRAN tape and the transitions the user has selected to include in the calculation.

BNDTRN BNDTRN translates the bands selected by the user to HITRAN nomenclature.

EWV EWV computes the equivalent width for a single isolated Voigt line.

LINRD This routine reads the binary line parameter file, one line at a time.

PRTROT This routine calculates the rotational partition function.

ROT ROT calculates the line-of-sight radiance for a pure rotational line.

ROTVIB ROTVIB calculates the line-of-sight radiance for a ro-vibrational line.

SPCRAD This is the spectral radiance routine and is called by the main SHARC routine. This routine calls LINRD to read an individual line, calls BNDCMP to determine if this line is for a user-selected transition, calls ROT/ROTVIB to perform the line-of-sight radiance calculation. The end result of this routine is the spectral radiance for a line which is stored in array RADBIN.

VIBES When ICHOIC=1 this routine converts 1982 vibrational assignments to 1985 format. When ICHOIC=2 the routine converts 1985 format to 1982 vibrational assignments. This routine is from the HITRAN line selection program.

OUTPUT Module

AMBOUT AMBOUT prints the atmospheric profile.

ATMOUT ATMOUT prints the atmospheric profile.

AUROUT AUROUT prints the time dependent number densities for an auroral calculation.

BANNER BANNER outputs the SHARC banner identifying the run.

BNDOUT This subroutine prints the line strength distribution function parameters.

BRDOUT — BRDOUT summarizes the calculated band radiances for each transition. The number of lines used in the radiance calculation is also printed.

GEMOUT — GEMOUT writes out a brief summary of the LOS information to SHARC.OUT.

GENOUT — GENOUT writes out a brief general description of each regional calculation.

NEMOUT — This subroutine prints out some of the inputs used by NEMESIS.

POPOUT — POPOUT outputs the number densities as a function of altitude for each vibrational state in the mechanism.

RADOUT — RADOUT outputs the information contained in the molecular states file.

RETOUT — RETOUT writes a summary of the population file to SHARC.OUT when an old population file is used in a new calculation.

SAVE — SAVE writes the population file.

SPCOUT — SPCOUT writes the spectral radiance as a function of wavenumber to SHARC.SPC.

SUMOUT — SUMOUT prints a calculational summary at the beginning of each SHARC run.

VBTOUT — VBTOUT outputs the vibrational temperatures as a function of altitude for each vibrational state in the mechanism.

VIBTMP — This routine calculates vibrational temperatures of excited-state species.

APPENDIX D

PLOTTING PACKAGE

The plotting software is a separate package which can be used to plot the spectral output of a SHARC computation. The program is written in Fortran 77. The program is designed to be as device independent as possible. It requires only standard Calcomp calls to initialize and terminated plotting, and a standard Calcomp call to move the pen. External routines which must be supplied by the user include INITPZ, ENDPLT and PPLT which are described below. All other aspects of plotting are device independent.

INITPZ — This subroutine initializes all system specific requirements for plotting and opens the plot file. Subroutine arguments are:

- PLTFIL - a character string which is the name of the plot file to be sent to the printer/plotter,
- NCPPLT - an integer equal to the number of characters in the plot file name,
- NPLT - the file unit number for the plot file.
- NERR - the file unit number for writing any error messages.

ENDPLT — ENDPLT terminates plotting and closes the plot files.

PPLT — PPLT draws a line or moves the pen to a new set of (X,Y) coordinates relative to the current origin. Subroutine arguments are:

- X - a real number giving the x position of the pen,
- Y - a real number giving the y position of the pen,
- IPEN - a pen control parameter. IPEN has the following meaning:

2	Lower pen and move
3	Raise pen and move
-2	Lower pen, move and reset origin to x,y
-3	Raise pen, move and reset origin to x,y